

# Density Matrix Expansion for Low-Momentum Interactions

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## Abstract

A first step toward a universal nuclear energy density functional based on low-momentum interactions is taken using the density matrix expansion (DME) of Negele and Vautherin. The DME is adapted for non-local momentum-space potentials and generalized to include local three-body interactions. Different prescriptions for the three-body DME are compared. Exploratory results are given at the Hartree-Fock level, along with a roadmap for systematic improvements within an effective action framework for Kohn-Sham density functional theory.

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## 1 Introduction

Calculating the properties of atomic nuclei from microscopic internucleon interactions is one of the most challenging and enduring problems of nuclear physics. However, recent developments in few- and many-body physics together with advances in computational technology give hope that controlled calculations of medium and heavy nuclei starting from a microscopic nuclear Hamiltonian will be forthcoming (see, for example, [1,2,3]). Density functional theory (DFT), which is a self-consistent framework that goes beyond conventional mean-field approaches, offers particular promise for medium to heavy nuclei. The central object in DFT is an energy functional of the nuclear densities that would apply to all the nuclides. Phenomenological functionals have

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had many successes but lack a microscopic foundation and theoretical control of errors, such that extrapolations to the limits of nuclear binding are uncontrolled.

Recent progress in evolving chiral effective field theory (EFT) interactions to lower momentum using renormalization group (RG) methods [4,5,6,7,8,9,10,11,12] (see also [13,14]) makes feasible a microscopic calculation of a universal nuclear energy density functional (UNEDF) [15]. The evolution weakens or largely eliminates sources of non-perturbative behavior in the two-nucleon sector such as strong short-range repulsion and the tensor force from iterated pion exchange [9], and the consistent three-nucleon interaction is perturbative at lower cutoffs [7]. When applied to nuclear matter, many-body perturbation theory for the energy appears convergent (at least in the particle-particle channel), with calculations that include most of the second-order contributions exhibiting saturation in nuclear matter and showing relatively weak dependence on the cutoff [8]. These features are favorable ingredients for a microscopic Kohn-Sham DFT treatment [16,17,18]. Indeed, Hartree-Fock is a reasonable (if not fully quantitative) starting point, which suggests that the theoretical developments and phenomenological successes of DFT for Coulomb interactions may be applicable to the nuclear case for low-momentum interactions.

A formal constructive framework for Kohn-Sham DFT based on effective actions of composite operators can be carried out using the inversion method [19,20,21,22,23,24,25,26]. This is an organization of the many-body problem that is based on calculating the response of a finite system to external, static sources rather than seeking the many-body wave function. It requires a tractable expansion (such as an EFT momentum expansion or many-body perturbation theory) that is controllable in the presence of inhomogeneous sources, which act as single-particle potentials. This is problematic for conventional internucleon interactions, for which the single-particle potential needs to be tuned to enhance the convergence of the hole-line expansion [27,28], but is ideally suited for low-momentum interactions. Given an expansion, one can construct a free-energy functional in the presence of the sources and then Legendre transform order-by-order to the desired functional of the densities. However, these are complicated, non-local functionals and we require functional derivatives with respect to the densities, whose dependences are usually only implicit. While this is a feasible program, it will require significant development to extend existing phenomenological nuclear DFT computer codes.

We seek a path that will be compatible in the short term with current nuclear DFT technology but testable and systematically improvable. In this regard, the phenomenological nuclear energy density functionals of the Skyrme form have the closest connection to low-momentum interactions. Modern Skyrme functionals have been applied over a very wide range of nuclei, with quantitative success in reproducing properties of nuclear ground states and low-lying

excitations [29,30,31]. Nevertheless, a significant reduction of the global and local errors is a major goal [32]. One strategy is to improve the functional itself; the form of the basic Skyrme functional in use is very restricted, consisting of a sum of local powers of various nuclear densities [e.g., see Eq. (1)]. Fits to measured nuclear data have given to date only limited constraints on possible density and isospin dependences and on the form of the spin-orbit interaction. Even qualitative insight into these properties from realistic microscopic calculations should be beneficial in improving the effectiveness of the energy density functional.

A theoretical connection of the Skyrme functional to free-space NN interactions was made long ago by Negele and Vautherin using the density matrix expansion (DME) [33,34,35], but there have been few subsequent microscopic developments. The DME originated as an expansion of the Hartree-Fock energy constructed using the nucleon-nucleon (NN) G matrix [33,34], which was treated in a local (i.e., diagonal in coordinate representation) approximation. In this paper, we revisit the DME using non-local low-momentum interactions in momentum representation, for which G matrix summations are not needed because of the softening of the interaction. When applied to a Hartree-Fock energy functional, the DME yields an energy functional in the form of a generalized Skyrme functional that is compatible with existing codes, by replacing Skyrme coefficients with density-dependent functions. As in the original application, a key feature of the DME is that it is not a pure short-distance expansion but includes resummations that treat long-range pion interactions correctly in a uniform system. However, we caution that the Negele-Vautherin DME involves prescriptions for the resummations without a corresponding power counting to justify them.

The idea of using soft, non-local potentials in an expansion starting with Hartree-Fock was explored in the late sixties and early seventies (see, for example, Refs. [36,37,38]). However, soft potentials were generally abandoned because of their inability to saturate nuclear matter at the empirical density and energy per particle.<sup>1</sup> They have been revived in the context of low-momentum potentials (often referred to as “ $V_{\text{low } k}$ ”) derived by transforming modern realistic NN potentials. The key to their success is the recognition that three-body forces (and possibly four-body forces) cannot be neglected. With lowered cutoffs, the density dependence of the three-body contribution drives saturation [8], which accounts for the apparent past failure in nuclear matter when only two-body contributions were included.

The present work is a proof-of-principle demonstration with a roadmap for future developments. We note the following omissions and simplifications.

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<sup>1</sup> Calculations using hard NN-only interactions also fail to reproduce empirical saturation properties.

- We restrict ourselves to isoscalar ( $N = Z$ ) functionals. This is merely for simplicity; generalizations to the full isovector dependence will be presented in the near future. We also defer inclusion of spin-orbit and tensor terms, which will require extensions of the DME treatment of Negele and Vautherin [39].
- We work to leading order in the perturbative many-body expansion (i.e., Hartree-Fock). An upgrade path to include second order and beyond is described in Section 6.
- The form for the three-body force is limited to that of chiral N<sup>2</sup>LO EFT. This is consistent with current approximations used with low-momentum potentials, but will need to be generalized to accommodate evolved three-body potentials.
- Pairing is essential for the quantitative treatment of nuclei, particularly unstable nuclei. The DME functionals described here can be adapted to include pairing as done in conventional Hartree-Fock-Bogoliubov phenomenology. However, a unified treatment is feasible with low-momentum interactions [40,41].
- There are unresolved conceptual issues for applying DFT to a self-bound system [42,43,44] that we will not address here (but which must be dealt with eventually). In addition, projection is not considered.

Recently, Kaiser and collaborators have applied the DME in momentum space to a perturbative chiral EFT expansion at finite density to derive a Skyrme-like energy functional for nuclei [45,46,47]. Their analytic expressions for long-range pion contributions can be effectively applied in our formalism to avoid slowly converging partial-wave summations. However, we defer to future work a detailed description of this application and also comparisons with their results.

The plan of the paper is as follows. In Section 2, we present the features of density functional theory needed in our treatment and discuss how applying the DME will lead us to a generalized Skyrme-like energy functional. In Section 3, we review the Negele/Vautherin derivation of the DME for non-local (in coordinate space) two-body potentials and make a direct extension to momentum space. The result is a set of simple formulas for the basic coefficient functions in terms of integrals over partial-wave matrix elements of the  $V_{\text{low } k}$  potential. In Section 4, we extend the DME to include three-body forces, restricting ourselves to local potentials of the form used in chiral EFT at N<sup>2</sup>LO (which is the form used in current approximations to low-momentum NNN interactions). We consider two prescriptions for the three-body part. We present some tests of the DME and sample results in Section 5, highlighting the effects of non-locality, the relative size of NN and NNN contributions, and the impact of different prescriptions for the NNN DME expansion. We conclude with a summary and roadmap for future calculations in Section 6.

## 2 Density Functional Theory

In this section, we give overviews of the standard Skyrme functional and the ideas behind Kohn-Sham DFT for nuclei that we need to set up the energy density functional calculations using the DME.

### 2.1 Skyrme Hartree-Fock Energy Density Functional

In the conventional Skyrme Hartree-Fock (SHF) formalism, the energy is a functional of the density  $\rho$ , the kinetic density  $\tau$ , and the spin-orbit density  $\mathbf{J}$ . For simplicity, we restrict the discussion to  $N = Z$  nuclei here, so these are isoscalar densities only. This functional is a single integral of a local energy density, which depends in a simple way on these densities, such as [48]

$$E_{\text{SHF}}[\rho, \tau, \mathbf{J}] = \int d^3x \left\{ \frac{1}{2M} \tau + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} t_3 \rho^{2+\alpha} + \frac{1}{16} (3t_1 + 5t_2) \rho \tau + \frac{1}{64} (9t_1 - 5t_2) (\nabla \rho)^2 - \frac{3}{4} W_0 \rho \nabla \cdot \mathbf{J} + \frac{1}{32} (t_1 - t_2) \mathbf{J}^2 \right\}. \quad (1)$$

Expressions for the Skyrme functional including isovector and more general densities can be found in Ref. [49]. The densities  $\rho$ ,  $\tau$ , and  $\mathbf{J}$  are expressed as sums over single-particle orbitals  $\phi_\beta(\mathbf{x})$ :

$$\rho(\mathbf{x}) \equiv \sum_{\beta} |\phi_\beta(\mathbf{x})|^2, \quad (2)$$

$$\tau(\mathbf{x}) \equiv \sum_{\beta} |\nabla \phi_\beta(\mathbf{x})|^2, \quad (3)$$

$$\mathbf{J}(\mathbf{x}) \equiv \sum_{\beta} \phi_\beta^\dagger(\mathbf{x}) (-i \nabla \times \boldsymbol{\sigma}) \phi_\beta(\mathbf{x}), \quad (4)$$

where the sums are over occupied states and the spin-isospin indices are implicit. (More generally, when pairing is included with a zero-range interaction, the sums are over all orbitals up to a cutoff, weighted by pairing occupation numbers. This complicates finding the self-consistent solution significantly but is not important for our discussion.) The parameters  $t_0$ – $t_3$ ,  $W_0$ , and  $\alpha$  determine the functional and are obtained from numerical fits to experimental data.

Varying the energy with respect to the wavefunctions with Lagrange multipliers  $\varepsilon_\beta$  to ensure normalization<sup>2</sup> leads to a Schrödinger-type equation with a

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<sup>2</sup> Unconstrained variation of the orbitals is the usual textbook formulation of

position-dependent mass term [50,48]:

$$\left(-\nabla \frac{1}{2M^*(\mathbf{x})} \nabla + U(\mathbf{x}) + \frac{3}{4}W_0 \nabla \rho \cdot \frac{1}{i} \nabla \times \boldsymbol{\sigma}\right) \phi_\beta(\mathbf{x}) = \varepsilon_\beta \phi_\beta(\mathbf{x}), \quad (5)$$

where [48]

$$U(\mathbf{x}) = \frac{3}{4}t_0\rho + \frac{3}{16}t_3\rho^2 + \frac{1}{16}(3t_1 + 5t_2)\tau + \frac{1}{32}(5t_2 - 9t_1)\nabla^2\rho - \frac{3}{4}W_0 \nabla \cdot \mathbf{J}, \quad (6)$$

the effective mass  $M^*(\mathbf{x})$  is

$$\frac{1}{2M^*(\mathbf{x})} = \frac{1}{2M} + \left[\frac{3}{16}t_1 + \frac{5}{16}t_2\right] \rho(\mathbf{x}), \quad (7)$$

and the  $W_0$  term is a spin-orbit potential (see Ref. [51] for details). The potentials in Eqs. (6)–(7) and the orbitals from Eq. (5) are evaluated alternately until self-consistency (see Fig. 10).

As we will see below, the DME energy functional for  $N = Z$  will take the same local form as  $E_{\text{SHF}}$ ,

$$E_{\text{DME}}[\rho, \tau, \mathbf{J}] = \int d^3R \mathcal{E}_{\text{DME}}(\rho(\mathbf{R}), \tau(\mathbf{R}), \mathbf{J}(\mathbf{R})), \quad (8)$$

where the energy density function  $\mathcal{E}_{\text{DME}}$  is evaluated with the local densities at  $\mathbf{R}$ . We follow the Negele/Vautherin notation for  $\mathcal{E}_{\text{DME}}$  and write [33]

$$\mathcal{E}_{\text{DME}} = \frac{\tau}{2M} + A[\rho] + B[\rho]\tau + C[\rho]|\nabla\rho|^2 + \dots, \quad (9)$$

where  $A$ ,  $B$ ,  $C$  are functions of the isoscalar density  $\rho$  instead of the constant Skyrme parameters, and we have suppressed terms that go beyond the present limited discussion. (When  $N \neq Z$ , these are functions of the isovector densities as well.) Equation (9) implies that the DME form will be a direct generalization of the Skyrme functionals.

## 2.2 DFT from Effective Actions

Microscopic DFT follows from calculating the response of a many-body system to external sources, as in Green's function methods, only with local, static sources that couple to densities rather than fundamental fields. (Time-dependent sources can be used for certain excited states.) It is profitable to

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Skyrme Hartree-Fock [48]. But this *does not* hold beyond Hartree level for a general microscopic DFT treatment with finite-range potentials, for which there is an additional constraint to the orbital variation [18].

think in terms of a thermodynamic formulation of DFT, which uses the effective action formalism [52] applied to composite operators to construct energy density functionals [19,20,22]. The basic plan is to consider the zero temperature limit of the partition function  $\mathcal{Z}$  for the (finite) system of interest in the presence of external sources coupled to various quantities of interest (such as the fermion density). We derive energy functionals of these quantities by Legendre transformations with respect to the sources [53]. These sources probe, in a variational sense, configurations near the ground state.

An analogous system would be a lattice of interacting spins, to which we apply an external source in the form of a magnetic field  $H$  [52]. The Helmholtz free energy  $F[H]$  is calculated as the energy in the presence of the magnetic field and we determine the magnetization by a derivative with respect to the field,  $M(H) = -\partial F[H]/\partial H$ . It is often useful to reverse the problem, and ask what external field produces a specified magnetization. This leads us to the Gibbs free energy  $G[M]$ , which we obtain by inverting  $M(H)$  to find  $H(M)$  and performing a Legendre transform:

$$G[M] = F[H] + H(M)M . \quad (10)$$

Because  $H = \partial G[M]/\partial M$  and  $H$  vanishes in the ground state,  $G$  is extremized in the ground state (and concavity tells us that it is a minimum). If  $H$  is an inhomogeneous source, the formalism is generalized by replacing partial derivatives by functional derivatives and performing a functional Legendre transform.

To derive density functional theory, we follow the same procedure, but with sources that adjust density distributions rather than spins. (We can either introduce a chemical potential or only consider variations that preserve net particle number. We implicitly assume the latter here.) Consider first the simplest case of a single external source  $J(\mathbf{x})$  coupled to the density operator  $\hat{\rho}(x) \equiv \psi^\dagger(x)\psi(x)$  in the partition function

$$\mathcal{Z}[J] = e^{-W[J]} \sim \text{Tr} e^{-\beta(\hat{H} + J\hat{\rho})} \sim \int \mathcal{D}[\psi^\dagger] \mathcal{D}[\psi] e^{-\int [\mathcal{L} + J\psi^\dagger\psi]} , \quad (11)$$

for which we can construct a path integral representation with Lagrangian  $\mathcal{L}$  [52]. (Note: because our treatment is schematic, for convenience we neglect normalization factors and take the inverse temperature  $\beta$  and the volume  $\Omega$  equal to unity in the sequel.) The static density  $\rho(\mathbf{x})$  in the presence of  $J(\mathbf{x})$  is

$$\rho(\mathbf{x}) \equiv \langle \hat{\rho}(\mathbf{x}) \rangle_J = \frac{\delta W[J]}{\delta J(\mathbf{x})} , \quad (12)$$

which we invert to find  $J[\rho]$  and then Legendre transform from  $J$  to  $\rho$ :

$$\Gamma[\rho] = -W[J] + \int d^3x J(\mathbf{x})\rho(\mathbf{x}) , \quad (13)$$

with

$$J(\mathbf{x}) = \frac{\delta\Gamma[\rho]}{\delta\rho(\mathbf{x})} \longrightarrow \left. \frac{\delta\Gamma[\rho]}{\delta\rho(\mathbf{x})} \right|_{\rho_{\text{gs}}(\mathbf{x})} = 0. \quad (14)$$

For static  $\rho(\mathbf{x})$ ,  $\Gamma[\rho]$  is proportional to the conventional Hohenberg-Kohn energy functional, which by Eq. (14) is extremized at the ground state density  $\rho_{\text{gs}}(\mathbf{x})$  (and thermodynamic arguments establish that it is a minimum [21]).<sup>3</sup>

We still need a way to carry out the inversion from  $\rho[J]$  to  $J[\rho]$ ; a general approach is the inversion method of Fukuda et al. [19,20]. The idea is to expand the relevant quantities in a hierarchy, labeled by a counting parameter  $\lambda$ ,

$$W[J, \lambda] = W_0[J] + \lambda W_1[J] + \lambda^2 W_2[J] + \dots, \quad (15)$$

$$J[\rho, \lambda] = J_0[\rho] + \lambda J_1[\rho] + \lambda^2 J_2[\rho] + \dots, \quad (16)$$

$$\Gamma[\rho, \lambda] = \Gamma_0[\rho] + \lambda \Gamma_1[\rho] + \lambda^2 \Gamma_2[\rho] + \dots, \quad (17)$$

treating  $\rho$  as order unity (which is the same as requiring that there are no corrections to the zero-order density), and match order by order in  $\lambda$  to determine the  $J_i$ 's and  $\Gamma_i$ 's. Zeroth order is a noninteracting system with potential  $J_0(x)$ :

$$\Gamma_0[\rho] = -W_0[J_0] + \int d^3x J_0(\mathbf{x})\rho(\mathbf{x}) \quad (18)$$

and

$$\rho(\mathbf{x}) = \frac{\delta W_0[J_0]}{\delta J_0(\mathbf{x})}. \quad (19)$$

Because  $\rho$  appears only at zeroth order, it is always specified from the non-interacting system according to Eq. (19); there are no corrections at higher order. This is the Kohn-Sham system with the same density as the fully interacting system.

What we have done is to use the freedom to split  $J$  into  $J_0$  and  $J - J_0$ , which is essentially the same as introducing a single-particle potential  $U$  and splitting the Hamiltonian according to  $H = (H_0 + U) + (V - U)$ . Typically  $U$  is chosen to accelerate (or even allow) convergence of a many-body expansion (e.g., the Bethe-Brueckner-Goldstone theory [27,54,28]). For DFT, we choose it to ensure that the *density* is unchanged, order by order. Thus, we need the flexibility in the many-body expansion to choose  $U$  without seriously degrading the convergence; such freedom is characteristic of low-momentum interactions. (Note: If there is a non-zero external potential, it is simply included with  $J_0$ .)

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<sup>3</sup> A Minkowski-space formulation of the effective action with time-dependent sources leads naturally to an RPA-like generalization of DFT that can be used to calculate properties of collective excitations.



We diagonalize  $W_0[J_0]$  by introducing Kohn-Sham orbitals  $\phi_i$  and eigenvalues  $\varepsilon_i$ ,

$$[-\nabla^2/2m - J_0(\mathbf{x})]\phi_i = \varepsilon_i\phi_i \quad (20)$$

so that

$$\rho(\mathbf{x}) = \sum_{i=1}^A |\phi_i(\mathbf{x})|^2. \quad (21)$$

Then  $W_0$  is equal to the sum of  $\varepsilon_i$ 's. The orbitals and eigenvalues are used to construct the Kohn-Sham Green's functions, which are used as the propagator lines in calculations the  $W_i[J_0]$  diagrams. Finally, we find  $J_0$  for the ground state by truncating the chain at  $\Gamma_{i_{\max}}$ ,

$$J_0 \rightarrow W_1 \rightarrow \Gamma_1 \rightarrow J_1 \rightarrow W_2 \rightarrow \Gamma_2 \rightarrow \cdots \rightarrow W_{i_{\max}} \rightarrow \Gamma_{i_{\max}} \quad (22)$$

and completing the self-consistency loop:

$$J_0(\mathbf{x}) = - \sum_{i>0}^{i_{\max}} J_i(\mathbf{x}) = \sum_{i>0}^{i_{\max}} \frac{\delta\Gamma_i[\rho]}{\delta\rho(\mathbf{x})} \equiv \frac{\delta\Gamma_{\text{int}}[\rho]}{\delta\rho(\mathbf{x})}. \quad (23)$$

Calculating the successive  $\Gamma_i$ 's, whose sum is directly proportional to the desired energy functional, is described in Refs. [20,21,55,23].

When transforming from  $W_i$  to  $\Gamma_i$ , there are additional diagrams that take into account the adjustment of the source to maintain the same density and also so-called anomalous diagrams (these are two-particle reducible). A general discussion and Feynman rules for these diagrams are given in Refs. [20,21,23]. These two types of contribution cancel up through N<sup>3</sup>LO in an EFT expansion with short-range forces using dimensional regularization [23], just as they do in the inversion method used long ago by Kohn, Luttinger, and Ward [56,57] to show the relationship of zero-temperature diagrammatic calculations to ones using the finite-temperature Matsubara formalism in the zero-temperature limit. In the present application of the DME approximation to the effective action DFT formalism, they also cancel and so are omitted entirely.

Note that even though solving for Kohn-Sham orbitals makes the approach look like a mean-field Hartree calculation, the approximation to the energy and density is *only* in the truncation of Eq. (23). It is a mean-field formalism in the sense of a conventional loop expansion, which is nonperturbative only in the background field while including further correlations perturbatively order-by-order in loops. The special feature of DFT is that the saddlepoint evaluation applies the condition that there are no corrections to the density. We emphasize that this is not ordinarily an appropriate expansion for inter-nucleon interactions; it is the special features of low-momentum interactions that make them suitable.

To generalize the energy functional to accommodate additional densities such as  $\tau$  and  $\mathbf{J}$ , we simply introduce an additional source coupled to each density.

$$\begin{aligned}
J_0(\mathbf{R}) &= - \text{[diagram: double line from R to a vertex, then a loop with a wavy line]} + \text{[diagram: double line from R to a vertex, then a loop with a wavy line and a self-energy loop]} + \dots \\
&= \text{[diagram: double line from R to a vertex, then a loop with a wavy line]} + \text{[diagram: double line from R to a vertex, then a loop with a wavy line and a self-energy loop]} + \dots
\end{aligned}$$

Fig. 1. Schematic representation of Eq. (27) for a local potential, where the double-line symbol denotes the  $(\delta\rho/\delta J_0)^{-1}$  term.

Thus, to generate a DFT functional of the kinetic-energy density as well as the density, add  $\eta(\mathbf{x}) \nabla\psi^\dagger \cdot \nabla\psi$  to the Lagrangian and Legendre transform to an effective action of  $\rho$  and  $\tau$  [25]:

$$\Gamma[\rho, \tau] = W[J, \eta] - \int d^3x J(\mathbf{x})\rho(\mathbf{x}) - \int d^3x \eta(\mathbf{x})\tau(\mathbf{x}) . \quad (24)$$

The inversion method results in two Kohn-Sham potentials,

$$J_0(\mathbf{x}) = \left. \frac{\delta\Gamma_{\text{int}}[\rho, \tau]}{\delta\rho(\mathbf{x})} \right|_\tau \quad \text{and} \quad \eta_0(\mathbf{x}) = \left. \frac{\delta\Gamma_{\text{int}}[\rho, \tau]}{\delta\tau(\mathbf{x})} \right|_\rho , \quad (25)$$

where  $\Gamma_{\text{int}} \equiv \Gamma - \Gamma_0$ . The Kohn-Sham equation is now [25]

$$\left[ -\nabla \frac{1}{M^*(\mathbf{x})} \nabla - J_0(\mathbf{x}) \right] \phi_i = \epsilon_i \phi_i , \quad (26)$$

with an effective mass  $1/2M^*(\mathbf{x}) \equiv 1/2M - \eta_0(\mathbf{x})$ , just like in Skyrme HF. Generalizing to the spin-orbit or other densities (including pairing [40]) proceeds analogously. We note that the variational principle implies that adding sources will always improve the effectiveness of the energy functional.

The Feynman diagrams for  $W_i$  will in general include multiple vertex points over which to integrate. Further, the dependence on the densities will not be explicit except when we have Hartree terms with a local potential (that is, a potential diagonal in coordinate representation). One way to proceed is to calculate the Kohn-Sham potentials using a functional chain rule, e.g.,

$$J_0(\mathbf{R}) = \frac{\delta\Gamma_{\text{int}}[\rho]}{\delta\rho(\mathbf{R})} = \int d\mathbf{y} \left( \frac{\delta\rho(\mathbf{R})}{\delta J_0(\mathbf{y})} \right)^{-1} \frac{\delta\Gamma_{\text{int}}[\rho]}{\delta J_0(\mathbf{y})} , \quad (27)$$

and steepest descent [21]. This is illustrated schematically for a local interaction in Fig. 1. We see that the Kohn-Sham potential is always just a function of  $\mathbf{R}$  but that the functional is very non-local. If zero-range interactions are used, these diagrams collapse into an expression for  $J_0(\mathbf{R})$  that has no internal vertices, but this is no longer true for diagrams with more than one interaction. Orbital-based methods take the chain rule in Eq. (27) one step

further, adding a functional derivative of the sources with respect to the  $\phi_i$ 's (and  $\varepsilon_i$ 's); see Refs. [18,58,59,60] for background on these calculations applied to electronic systems. Eventually, we plan to carry out such calculations to construct the full energy density functional.

An alternative in the short term is to approximate  $W_{\text{int}}$  so that the dependence on the densities (rather than the sources or the orbitals) is explicit. This has two effects: the construction of the  $\Gamma_i$  from the  $W_i$  does not have additional terms and the necessary functional derivatives are immediate. An example of such an approach is the local density approximation (LDA). Here we go beyond the LDA with the density matrix expansion (DME). By expanding the  $W_i$  about a “center-of-mass”  $\mathbf{R}$ , we generate a local energy density that is a function of densities ( $\rho, \tau, \dots$ ) at  $\mathbf{R}$ . We choose sources to match these densities and carry out the Legendre transformation implicitly; the end result at leading order is calculating  $W_1$  using density matrices built from Kohn-Sham orbitals. We are able to vary with respect to the orbitals because the constraint of a multiplicative Kohn-Sham potential is built in. Then the resulting Kohn-Sham DFT has precisely the form of the Skyrme Hartree-Fock energy functional and single-particle equations.

### 2.3 Low-Momentum Potentials

The original DME application was based on a Hartree-Fock energy functional calculated with a G matrix, following the Brueckner-Bethe-Goldstone (BBG) method [27,54,28]. The latter involves infinite resummations of diagrams for nuclear many-body theory, as needed to deal with strongly repulsive potentials. In BBG there are two general resummations: the ladder diagrams into a G matrix and the hole-line expansion using the G matrix. Furthermore, to accelerate convergence of the hole-line expansion one needs to carefully choose a single-particle potential. This is problematic for the success of a Kohn-Sham DFT construction, for which the background field (which acts as a single-particle potential) has a separate constraint, namely to maintain the fermion density distribution.

Renormalization group (RG) methods can be used to evolve realistic nucleon-nucleon potentials (e.g., chiral EFT potentials at  $N^3\text{LO}$ ), which typically have strong coupling between high and low momentum (i.e., off-diagonal matrix elements of the potential in momentum representation are substantial), to derive low-momentum potentials in which high and low momentum parts are decoupled. This can be accomplished by lowering a momentum cutoff  $\Lambda$  [4,5,6,7] or performing a series of unitary transformations that drive the hamiltonian toward the diagonal [10,11,12]. The UCOM transformations of Ref. [13] is an alternative to explicit RG methods. In all cases, we have a potential for which

only low momenta contribute to low-energy nuclear observables, such as the binding energy of nuclei. For convenience, we'll refer to any of these as  $V_{\text{low } k}$ .

We stress that evolving  $V_{\text{low } k}$  does not lose relevant information for low-energy physics, which includes nuclear ground states and low-lying excitations, as long as the leading many-body interactions are kept [11]. The long-range physics, which is from pion exchange (and Coulomb), is preserved and remains local, while relevant short-range physics is encoded in the low-momentum potential through the RG evolution. Most important, for any  $V_{\text{low } k}$  potential the obstacles from strongly repulsive potentials are removed. Hartree-Fock (including three-body interactions) saturates nuclear matter and G matrix resummations are not required (but may still be advantageous). Thus, we have a hierarchy suitable for DFT based on many-body perturbation theory. [Note: While the need for particle-hole resummations remains to be investigated for  $V_{\text{low } k}$  potentials, results from the analogous UCOM potentials indicate perturbative particle-hole contributions for the energy [14].]

While the evolution of  $V_{\text{low } k}$  potentials does not disturb the locality of initial long-range potentials, the short-range part becomes increasingly non-local. That is, in coordinate representation  $\langle \mathbf{r} | V | \mathbf{r}' \rangle$  has an increasing range in  $|\mathbf{r} - \mathbf{r}'|$ . Thus we must test that the DME is a good expansion for such non-localities.

The interactions must include three-body (and higher-body) potentials, which should be consistently evolved with the two-body potential. These are not yet available (although SRG methods show promise of providing them in the near future [10,11,12]), and are instead approximated by adjusted chiral N<sup>2</sup>LO three-body potentials [7]. The validity of this approximation relies on the RG methods modifying only the short-distance part of the potential and is supported by the observation that the EFT hierarchy of many-body forces appears to be preserved by the RG running [7]. The N<sup>2</sup>LO three-body potentials are local and we restrict our present investigation for now to this option. Given this microscopic NN and NNN input, we apply the density matrix expansion to derive an energy density functional of the Skyrme form.

### 3 DME for Two-Body Potentials in Momentum Space

In this section we derive the density matrix expansion for a microscopic DFT starting from low-momentum (and non-local) two-body potentials. From Section 2.2, the relevant object we need to expand is  $W_{\text{int}}$ , which is expressed in terms of the Kohn-Sham orbitals and eigenvalues that comprise the Kohn-Sham single-particle propagators. For Hartree-Fock contributions of the form in Fig. 2(a), however, only the orbitals enter because the Kohn-Sham Green's function reduces to the density matrix. Similarly, higher-order contributions

such as the ladder diagrams in the particle-particle (pp) channel can also be put approximately into this form by averaging over the state dependence arising from the intermediate-state energy denominators. Therefore, while the results in this section are derived for the Hartree-Fock contributions to the functional, they can easily be generalized to include higher-order ladder contributions; this will be explored in a future publication.

In essence, the DME maps the orbital-dependent expressions for contributions to  $W_{\text{int}}$  of the type in Fig. 2(a) into a quasi-local form, with explicit dependence on the local densities  $\rho(\mathbf{R})$ ,  $\tau(\mathbf{R})$ ,  $\nabla^2\rho(\mathbf{R})$ , and so on. This greatly simplifies the determination of the Kohn-Sham potential because the functional derivatives of  $\Gamma_{\text{int}}$  can be evaluated directly.

### 3.1 Expression for $W_{\text{HF}}$

Before presenting the details of the DME derivation and its application to non-local low-momentum interactions, it is useful to first derive in some detail the starting expression for  $W_{\text{HF}}$ , the Hartree-Fock contribution to  $W_{\text{int}}$ . This will serve to introduce our basic notation and to highlight the differences between most existing DME studies, which are formulated with local interactions and in coordinate space throughout, and the current approach, which is formulated in momentum space and geared towards non-local potentials.

For a local potential, the distinction between the direct (Hartree) and exchange (Fock) contributions is significant, and is reflected in the conventional decomposition of the DFT energy functional for Coulomb systems, which separates out the Hartree piece. For a non-local potential, the distinction is blurred because the Hartree contribution now involves the density matrix (as opposed to the density) and it is not useful to make this separation when the range of the interaction is comparable to the non-locality.<sup>4</sup> Consequently, throughout this section we work instead with an antisymmetrized interaction.

For a general (i.e., non-local) free-space two-body potential  $\hat{V}$ ,  $W_{\text{HF}}$  is defined in terms of Kohn-Sham states [Eq. (20)] labeled by  $i$  and  $j$ ,

$$W_{\text{HF}} = \frac{1}{2} \sum_{ij}^A \langle ij | \hat{V} (1 - P_{12}) | ij \rangle = \frac{1}{2} \sum_{ij}^A \langle ij | \hat{\mathcal{V}} | ij \rangle. \quad (28)$$

The summation is over the occupied states and the antisymmetrized interaction  $\hat{\mathcal{V}} = \hat{V}(1 - P_{12})$  has been introduced, with the exchange operator

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<sup>4</sup> However, it is useful to separate out the long-distance part of the potential, which is local, and treat its direct (Hartree) contribution exactly.

$P_{12}$  equal to the product of operators for spin, isospin, and space exchange,  $P_{12} = P_\sigma P_\tau P_r$ . Note that the dependence of  $W_{\text{HF}}$  on the Kohn-Sham potential has been suppressed. By making repeated use of the completeness relation

$$11 = \sum_{\sigma\tau} \int d\mathbf{r} |\mathbf{r}\sigma\tau\rangle \langle \mathbf{r}\sigma\tau| , \quad (29)$$

$W_{\text{HF}}$  can be written in terms of the coordinate space Kohn-Sham orbitals as

$$\begin{aligned} W_{\text{HF}} = & \frac{1}{2} \sum_{ij} \sum_{\{\sigma\tau\}} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \int d\mathbf{r}_3 \int d\mathbf{r}_4 \langle \mathbf{r}_1 \sigma_1 \tau_1 \mathbf{r}_2 \sigma_2 \tau_2 | \hat{\mathcal{V}} | \mathbf{r}_3 \sigma_3 \tau_3 \mathbf{r}_4 \sigma_4 \tau_4 \rangle \\ & \times \phi_i^*(\mathbf{r}_1 \sigma_1 \tau_1) \phi_i(\mathbf{r}_3 \sigma_3 \tau_3) \phi_j^*(\mathbf{r}_2 \sigma_2 \tau_2) \phi_j(\mathbf{r}_4 \sigma_4 \tau_4) . \end{aligned} \quad (30)$$

From the definition of the Kohn-Sham density matrix,

$$\rho(\mathbf{r}_3 \sigma_3 \tau_3, \mathbf{r}_1 \sigma_1 \tau_1) = \sum_i^A \phi_i^*(\mathbf{r}_1 \sigma_1 \tau_1) \phi_i(\mathbf{r}_3 \sigma_3 \tau_3) , \quad (31)$$

so Eq. (30) can be written as

$$\begin{aligned} W_{\text{HF}} = & \frac{1}{2} \sum_{\{\sigma\tau\}} \int d\mathbf{r}_1 \cdots \int d\mathbf{r}_4 \langle \mathbf{r}_1 \sigma_1 \tau_1 \mathbf{r}_2 \sigma_2 \tau_2 | \hat{\mathcal{V}} | \mathbf{r}_3 \sigma_3 \tau_3 \mathbf{r}_4 \sigma_4 \tau_4 \rangle \\ & \times \rho(\mathbf{r}_3 \sigma_3 \tau_3, \mathbf{r}_1 \sigma_1 \tau_1) \rho(\mathbf{r}_4 \sigma_4 \tau_4, \mathbf{r}_2 \sigma_2 \tau_2) \\ = & \frac{1}{2} \text{Tr}_1 \text{Tr}_2 \int d\mathbf{r}_1 \cdots \int d\mathbf{r}_4 \langle \mathbf{r}_1 \mathbf{r}_2 | \mathcal{V}^{1\otimes 2} | \mathbf{r}_3 \mathbf{r}_4 \rangle \boldsymbol{\rho}^{(1)}(\mathbf{r}_3, \mathbf{r}_1) \boldsymbol{\rho}^{(2)}(\mathbf{r}_4, \mathbf{r}_2) , \end{aligned} \quad (32)$$

where a matrix notation is used in the second equation and the traces denote summations over the spin and isospin indices for “particle 1” and “particle 2”. Hereafter we drop the superscripts on  $\mathcal{V}$  and  $\boldsymbol{\rho}$  that indicate which space they act in as it will be clear from the context.

Expanding the  $\boldsymbol{\rho}$  matrices on Pauli spin and isospin matrices we have

$$\boldsymbol{\rho}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{4} [\rho_0(\mathbf{r}_1, \mathbf{r}_2) + \rho_1(\mathbf{r}_1, \mathbf{r}_2) \tau_z + \vec{S}_0(\mathbf{r}_1, \mathbf{r}_2) \cdot \vec{\sigma} + \vec{S}_1(\mathbf{r}_1, \mathbf{r}_2) \cdot \vec{\sigma} \tau_z] , \quad (33)$$

where we have assumed the absence of charge-mixing in the single-particle states. The usual scalar-isoscalar, scalar-isovector, vector-isoscalar, and vector-isovector components are obtained by taking the relevant traces,

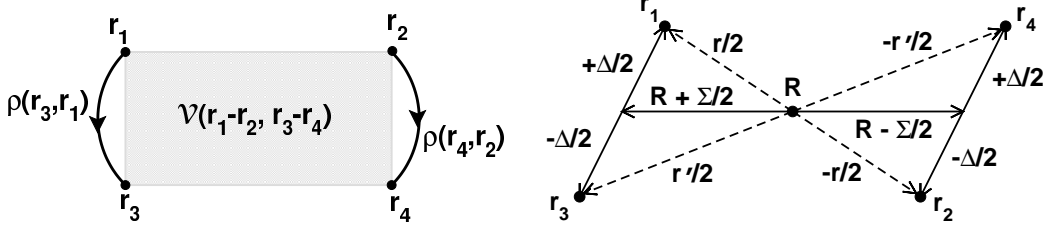


Fig. 2. (a) Schematic diagram for approximations to  $W_{\text{int}}$  that can be expanded using the DME. (b) Coordinates appropriate for the DME applied to the Hartree-Fock potential energy with a non-local potential.

$$\rho_0(\mathbf{r}_1, \mathbf{r}_2) \equiv \text{Tr}_{\sigma\tau}[\boldsymbol{\rho}(\mathbf{r}_1, \mathbf{r}_2)] = \sum_i^A \phi_i^\dagger(\mathbf{r}_2) \phi_i(\mathbf{r}_1) , \quad (34)$$

$$\rho_1(\mathbf{r}_1, \mathbf{r}_2) \equiv \text{Tr}_{\sigma\tau}[\boldsymbol{\rho}(\mathbf{r}_1, \mathbf{r}_2) \tau_z] = \sum_i^A \phi_i^\dagger(\mathbf{r}_2) \tau_z \phi_i(\mathbf{r}_1) , \quad (35)$$

$$\vec{S}_0(\mathbf{r}_1, \mathbf{r}_2) \equiv \text{Tr}_{\sigma\tau}[\boldsymbol{\rho}(\mathbf{r}_1, \mathbf{r}_2) \vec{\sigma}] = \sum_i^A \phi_i^\dagger(\mathbf{r}_2) \vec{\sigma} \phi_i(\mathbf{r}_1) , \quad (36)$$

$$\vec{S}_1(\mathbf{r}_1, \mathbf{r}_2) \equiv \text{Tr}_{\sigma\tau}[\boldsymbol{\rho}(\mathbf{r}_1, \mathbf{r}_2) \vec{\sigma} \tau_z] = \sum_i^A \phi_i^\dagger(\mathbf{r}_2) \vec{\sigma} \tau_z \phi_i(\mathbf{r}_1) , \quad (37)$$

where  $\phi_i(\mathbf{r})$  denotes a spinor with components  $\phi_i(\mathbf{r}\sigma\tau)$ .

In this initial work we will only consider terms in the energy functional arising from products of the scalar-isoscalar ( $\rho_0$ ) density matrices in Eq. (32), which are the relevant terms for spin-saturated systems with  $N = Z$ . Thus, we will drop the subscript “0” on the density matrices from now on.

After switching to relative/center-of-mass (COM) coordinates (see Fig. 2) and noting that the free-space two-nucleon potential is diagonal in the COM coordinate, the starting point for our DME of the two-body Hartree-Fock contribution from a non-local interaction is

$$W_{\text{HF}} = \frac{1}{32} \int d\mathbf{R} d\mathbf{r} d\mathbf{r}' \rho(\mathbf{R} + \frac{\mathbf{r}'}{2}, \mathbf{R} + \frac{\mathbf{r}}{2}) \rho(\mathbf{R} - \frac{\mathbf{r}'}{2}, \mathbf{R} - \frac{\mathbf{r}}{2}) \text{Tr}_{\sigma\tau}[\langle \mathbf{r} | \mathbf{V} | \mathbf{r}' \rangle] , \quad (38)$$

where  $\mathbf{V}$  denotes the antisymmetrized interaction and the trace is defined as

$$\text{Tr}_{\sigma\tau}[\langle \mathbf{r} | \mathbf{V} | \mathbf{r}' \rangle] \equiv \sum_{\{\sigma\tau\}} \langle \mathbf{r} \sigma_1 \tau_1 \sigma_2 \tau_2 | \hat{V} (1 - P_{12}) | \mathbf{r}' \sigma_1 \tau_1 \sigma_2 \tau_2 \rangle . \quad (39)$$

The DME derivation of Negele and Vautherin (NV) [33] focuses on applications to local potentials, which satisfy  $\langle \mathbf{r} | \hat{V} | \mathbf{r}' \rangle = \delta(\mathbf{r} - \mathbf{r}') \langle \mathbf{r} | \hat{V} | \mathbf{r}' \rangle$ . While the original NV work included coordinate-space formulas applicable for non-local

interactions<sup>5</sup>, for low-momentum potentials it is convenient to revisit and extend the original derivation to a momentum-space formulation. We note that Kaiser et al. have shown how to use medium-insertions in momentum space in their application of the DME to chiral perturbation theory at finite density [45,46,47].

For the momentum space formulation, we first rewrite the density matrices appearing in Eq. (38) as

$$\rho(\mathbf{R} \pm \mathbf{r}'/2, \mathbf{R} \pm \mathbf{r}/2) = \rho(\mathbf{R}^\pm \pm \mathbf{\Delta}/2, \mathbf{R}^\pm \mp \mathbf{\Delta}/2) , \quad (40)$$

where the vectors appearing on the right-hand side are defined by (see Fig. 2)

$$\mathbf{R}^\pm = \mathbf{R} \pm \frac{1}{2}\mathbf{\Sigma} , \quad \mathbf{\Sigma} = \frac{1}{2}(\mathbf{r}' + \mathbf{r}) , \quad \mathbf{\Delta} = \frac{1}{2}(\mathbf{r}' - \mathbf{r}) . \quad (41)$$

Introducing the Fourier transform of  $\mathbf{V}$  in the momentum transfers conjugate to  $\mathbf{\Sigma}$  and  $\mathbf{\Delta}$ ,

$$\mathbf{q} = \mathbf{k} - \mathbf{k}' , \quad \mathbf{p} = \mathbf{k} + \mathbf{k}' , \quad (42)$$

(where  $\mathbf{k}'$ ,  $\mathbf{k}$  correspond to relative momenta) gives

$$W_{\text{HF}} = \frac{1}{32} \int d\mathbf{R} \int \frac{d\mathbf{q} d\mathbf{p}}{(2\pi)^6} F(\mathbf{R}, \mathbf{q}, \mathbf{p}) \text{Tr}_{\sigma\tau}[\tilde{\mathbf{V}}(\mathbf{q}, \mathbf{p})] , \quad (43)$$

where we have defined

$$F(\mathbf{R}, \mathbf{q}, \mathbf{p}) \equiv \int d\mathbf{\Sigma} d\mathbf{\Delta} e^{i\mathbf{q}\cdot\mathbf{\Sigma}} e^{i\mathbf{p}\cdot\mathbf{\Delta}} \rho(\mathbf{R}^+ - \mathbf{\Delta}/2, \mathbf{R}^+ + \mathbf{\Delta}/2) \\ \times \rho(\mathbf{R}^- + \mathbf{\Delta}/2, \mathbf{R}^- - \mathbf{\Delta}/2) , \quad (44)$$

and

$$\tilde{\mathbf{V}}(\mathbf{q}, \mathbf{p}) \equiv 8 \int d\mathbf{\Sigma} d\mathbf{\Delta} e^{-i\mathbf{q}\cdot\mathbf{\Sigma}} e^{-i\mathbf{p}\cdot\mathbf{\Delta}} \langle \mathbf{\Sigma} - \mathbf{\Delta} | \mathbf{V} | \mathbf{\Sigma} + \mathbf{\Delta} \rangle . \quad (45)$$

The momenta  $\mathbf{q}$  and  $\mathbf{p}$  correspond to the momentum transfers for a local interaction in the direct and exchange channels. That is, the direct matrix element is a function of  $\mathbf{q}$  and the exchange is a function of  $\mathbf{p}$ . In contrast, for a non-local interaction the direct and exchange matrix elements depend on both  $\mathbf{q}$  and  $\mathbf{p}$ . This is the reason why we do not attempt to separate out the Hartree (direct) and Fock (exchange) contributions to  $W_{\text{HF}}$ , as is commonly done for local interactions.

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<sup>5</sup> However, note that the final formulas for non-local potentials in Ref. [33] have numerous errors, which were not among those corrected in Ref. [34].



The trace of Eq. (45) can be written in a more convenient form for our purposes as a sum over partial wave matrix elements,

$$\text{Tr}_{\sigma\tau}[\tilde{\mathcal{V}}(\mathbf{q}, \mathbf{p})] = 8\pi \sum_{lsj}' (2j+1)(2t+1) P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}') \langle klsjt|V|k'lsjt\rangle, \quad (46)$$

where the primed summation means that it is restricted to values where  $l+s+t$  is odd, with  $\mathbf{k} = \frac{1}{2}(\mathbf{p} + \mathbf{q})$  and  $\mathbf{k}' = \frac{1}{2}(\mathbf{p} - \mathbf{q})$ . For simplicity we have assumed a charge-independent two-nucleon interaction, although charge-dependence can easily be included.

### 3.2 Density Matrix Expansion

The expression Eq. (43) for  $W_{\text{HF}}$  is written in terms of off-diagonal density matrices constructed from the Kohn-Sham orbitals. Consequently, the corresponding  $\Gamma_{\text{HF}}[\rho]$  is an *implicit* functional of the density. The orbital-dependent  $\Gamma_{\text{HF}}$  requires the use of the functional derivative chain rule to evaluate  $J_1(\mathbf{R}) = \delta\Gamma_{\text{HF}}[\rho]/\delta\rho(\mathbf{R})$  in the self-consistent determination of the Kohn-Sham potential, which presents computational challenges and would require substantial enhancements to existing Skyrme HFB codes.

Alternatively, we can apply Negele and Vautherin's DME to  $W_{\text{HF}}$ , resulting in an expression as in Eq. (9) with *explicit* dependence on the local quantities  $\rho(\mathbf{R})$ ,  $\tau(\mathbf{R})$ , and  $|\nabla\rho(\mathbf{R})|^2$ ,

$$W_{\text{HF}} = \int d\mathbf{R} (A[\rho] + B[\rho]\tau + C[\rho](\nabla\rho)^2 + \dots). \quad (47)$$

The starting point of the DME is the formal identity [33]

$$\begin{aligned} \rho(\mathbf{R} + \mathbf{s}/2, \mathbf{R} - \mathbf{s}/2) &= \sum_a \phi^*(\mathbf{R} + \mathbf{s}/2) \phi(\mathbf{R} - \mathbf{s}/2) \\ &= \left[ e^{\mathbf{s} \cdot (\nabla_1 - \nabla_2)/2} \sum_a \phi^*(\mathbf{R}_1) \phi(\mathbf{R}_2) \right]_{\mathbf{R}_1 = \mathbf{R}_2 = \mathbf{R}}, \end{aligned} \quad (48)$$

where  $\nabla_1$  and  $\nabla_2$  act on  $\mathbf{R}_1$  and  $\mathbf{R}_2$ , respectively, and the result is evaluated at  $\mathbf{R}_1 = \mathbf{R}_2 = \mathbf{R}$ . We assume here that time-reversed orbitals are filled pairwise, so that the linear term of the exponential expansion vanishes. Hence, through second-order gradient terms the angular integral of the density matrix squared is equivalent to the integral of the square of the angle-averaged density matrix. In this way, the leading off-diagonal behavior of the density matrices in  $W_{\text{HF}}$  is captured by simpler expressions.

The angle-averaged density matrix takes the form

$$\begin{aligned}\hat{\rho}(\mathbf{R} + \mathbf{s}/2, \mathbf{R} - \mathbf{s}/2) &= \frac{1}{2} \int d\cos\theta \exp[\mathbf{s} \cdot (\nabla_1 - \nabla_2)/2] \rho(\mathbf{R}_1, \mathbf{R}_2) \\ &= \frac{\sinh[\frac{1}{2}s|\nabla_1 - \nabla_2|]}{\frac{1}{2}s|\nabla_1 - \nabla_2|} \rho(\mathbf{R}_1, \mathbf{R}_2) \Big|_{\mathbf{R}_1=\mathbf{R}_2=\mathbf{R}},\end{aligned}\quad (49)$$

with  $s \equiv |\mathbf{s}|$ . Using a Bessel-function expansion (which is simply the usual plane-wave expansion with real arguments),

$$\frac{1}{xy} \sinh(xy) = \frac{1}{x} \sum_{k=0}^{\infty} (-1)^k (4k+3) j_{2k+1}(x) \mathcal{Q}_k(y^2), \quad (50)$$

where  $\mathcal{Q}$  is related to the usual Legendre polynomial by  $\mathcal{Q}(z^2) = P_{2k+1}(iz)/(iz)$ , we can express the angle-averaged density matrix as

$$\begin{aligned}\hat{\rho}(\mathbf{R} + \mathbf{s}/2, \mathbf{R} - \mathbf{s}/2) &= \frac{1}{sk_F(\mathbf{R})} \left[ \sum_{n=0}^{\infty} (4n+3) j_{2n+1}(sk_F(\mathbf{R})) \right. \\ &\quad \left. \times \mathcal{Q}_n\left(\left(\frac{\nabla_1 - \nabla_2}{2k_F(\mathbf{R})}\right)^2\right) \right] \rho(\mathbf{R}_1, \mathbf{R}_2),\end{aligned}\quad (51)$$

where an arbitrary momentum scale  $k_F(\mathbf{R})$  has been introduced. Equation (51) is independent of  $k_F$  if all terms are kept, but any truncation will give results depending on the particular choice for  $k_F$ . In this initial study, we employ the standard LDA choice of Negele and Vautherin:

$$k_F(\mathbf{R}) = (3\pi^2 \rho(\mathbf{R})/2)^{1/3}. \quad (52)$$

Alternative choices for  $k_F(\mathbf{R})$  to optimize the convergence of truncated expansions of Eq. (51) and to establish a power counting will be explored in a future paper.

Following Negele and Vautherin, Eq. (51) is truncated to terms with  $n \leq 1$ , which yields the fundamental equation of the DME,

$$\begin{aligned}\hat{\rho}(\mathbf{R} + \frac{\mathbf{s}}{2}, \mathbf{R} - \frac{\mathbf{s}}{2}) &\approx \rho_{\text{SL}}(k_F(\mathbf{R})s) \rho(\mathbf{R}) \\ &\quad + s^2 g(k_F(\mathbf{R})s) \left[ \frac{1}{4} \nabla^2 \rho(\mathbf{R}) - \tau(\mathbf{R}) + \frac{3}{5} k_F(\mathbf{R})^2 \rho(\mathbf{R}) \right],\end{aligned}\quad (53)$$

where

$$\rho_{\text{SL}}(x) \equiv 3j_1(x)/x, \quad g(x) \equiv 35j_3(x)/2x^3, \quad (54)$$

and the kinetic energy density is  $\tau(\mathbf{R}) = \sum_i |\nabla \phi_i(\mathbf{R})|^2$ . If a short-range interaction is folded with the density matrix, then a truncated Taylor series expansion of Eq. (53) in powers of  $s$  would be justified and would produce

a quasi-local functional. But the local  $k_F$  in the interior of a nucleus is typically greater than the pion mass  $m_\pi$ , so such an expansion would give a poor representation of the physics of the long-range pion exchange interaction.

Instead, the DME is constructed as an expansion about the exact nuclear matter density matrix. Thus, Eq. (53) has the important feature that it reduces to the density matrix in the homogenous nuclear matter limit,  $\rho_{\text{NM}}(\mathbf{R} + \mathbf{s}/2, \mathbf{R} - \mathbf{s}/2) = \rho_{\text{SL}}(k_F s) \rho$ . As a result, the resummed expansion in Eq. (53) does not distort the finite range physics, as the long-range one-pion-exchange contribution to nuclear matter is exactly reproduced and the finite-range physics is encoded as non-trivial (e.g., non-monomial) density dependence in the resulting functional. The small parameters justifying this expansion emerge in the functionals as integrals over the inhomogeneities of the density. (See Ref. [24] for examples of estimated contributions to a functional for a model problem.)

In the case of a local interaction, the Fock term is schematically given by  $W_F \sim \int d\mathbf{R} d\mathbf{s} \rho^2(\mathbf{R} + \mathbf{s}/2, \mathbf{R} - \mathbf{s}/2) V(\mathbf{s})$ , so a single application of Eq. (53) is sufficient to cast  $W_{\text{HF}}$  into the desired form. For a non-local interaction the calculation is more involved as two applications of the DME are required. Following Negele and Vautherin, we first rewrite the density matrices appearing in Eq. (38) as

$$\rho(\mathbf{R} \pm \mathbf{r}'/2, \mathbf{R} \pm \mathbf{r}/2) = \rho(\mathbf{R}^\pm \pm \Delta/2, \mathbf{R}^\pm \mp \Delta/2), \quad (55)$$

where the vectors appearing on the right-hand side are defined by (see Fig. 2)

$$\mathbf{R}^\pm \equiv \mathbf{R} \pm \frac{1}{2}\Sigma, \quad \Sigma \equiv \frac{1}{2}(\mathbf{r}' + \mathbf{r}), \quad \Delta \equiv \frac{1}{2}(\mathbf{r}' - \mathbf{r}). \quad (56)$$

To simplify the notation we define

$$k_F^\pm \equiv k_F(\mathbf{R}^\pm), \quad \rho^\pm \equiv \rho(\mathbf{R}^\pm), \quad \tau^\pm \equiv \tau(\mathbf{R}^\pm), \quad (57)$$

and it is from now on understood that the functions without superscripts depend only on the center-of-mass vector  $\mathbf{R}$  if the argument is not written explicitly.

The first application of the DME corresponds to an expansion in the non-locality  $\Delta$  about the “shifted” COM coordinates  $\mathbf{R}^\pm$ , giving

$$\begin{aligned} \rho(\mathbf{R} + \mathbf{r}'/2, \mathbf{R} + \mathbf{r}/2) &= \rho(\mathbf{R}^+ - \Delta/2, \mathbf{R}^+ + \Delta/2) \\ &\approx \rho_{\text{SL}}(k_F^+ \Delta) \rho^+ + \Delta^2 g(k_F^+ \Delta) \left[ \frac{1}{4} \nabla^2 \rho^+ - \tau^+ + \frac{3}{5} k_F^{+2} \rho^+ \right]. \end{aligned} \quad (58)$$

Thus, we can expand the product of density matrices in Eq. (38) as

$$\begin{aligned}
\rho(\mathbf{R} + \frac{\mathbf{r}'}{2}, \mathbf{R} + \frac{\mathbf{r}}{2}) \rho(\mathbf{R} - \frac{\mathbf{r}'}{2}, \mathbf{R} - \frac{\mathbf{r}}{2}) &= \rho_{\text{SL}}(k_{\text{F}}^+ \Delta) \rho^+ \rho_{\text{SL}}(k_{\text{F}}^- \Delta) \rho^- \\
&+ \Delta^2 g(k_{\text{F}}^+ \Delta) \rho_{\text{SL}}(k_{\text{F}}^- \Delta) \rho^- \left[ \frac{1}{4} \nabla^2 \rho^+ - \tau^+ + \frac{3}{5} k_{\text{F}}^{+2} \rho^+ \right] \\
&+ \Delta^2 g(k_{\text{F}}^- \Delta) \rho_{\text{SL}}(k_{\text{F}}^+ \Delta) \rho^+ \left[ \frac{1}{4} \nabla^2 \rho^- - \tau^- + \frac{3}{5} k_{\text{F}}^{-2} \rho^- \right], \quad (59)
\end{aligned}$$

where we have dropped terms quadratic in the gradient. We then define

$$\alpha(\rho^\pm) = \rho_{\text{SL}}(k_{\text{F}}^\pm \Delta) \rho^\pm, \quad (60)$$

and use Eq. (50) to perform a *second* density matrix expansion on  $\alpha(\rho^+) \alpha(\rho^-)$  in  $\Sigma$  about  $\mathbf{R}$ ,

$$\alpha(\rho^+) \alpha(\rho^-) \approx \rho_{\text{SL}}(k_{\text{F}} \Sigma) \alpha^2 + \frac{\Sigma^2}{2} g(k_{\text{F}} \Sigma) [\alpha \nabla^2 \alpha - |\nabla \alpha|^2 + \frac{6}{5} k_{\text{F}}^2 \alpha^2]. \quad (61)$$

From a Taylor expansion of  $\rho_{\text{SL}}(k_{\text{F}} \Sigma)$  and  $g(k_{\text{F}} \Sigma)$  it is evident that the  $(k_{\text{F}} \Sigma)^2$  coefficients of  $\alpha^2$  exactly cancel each other. Because we desire a final expression that reproduces the exact nuclear matter limit (and the presence of the  $\rho_{\text{SL}}(k_{\text{F}} \Sigma)$  term spoils this limit), we follow the philosophy of Negele and Vautherin and use this leading cancellation to motivate a different rearrangement and truncation of Eq. (51) such that

$$\alpha(\rho^+) \alpha(\rho^-) \approx \alpha^2 + \frac{\Sigma^2}{2} g(k_{\text{F}} \Sigma) [\alpha \nabla^2 \alpha - |\nabla \alpha|^2]. \quad (62)$$

The freedom to rearrange the expansion as in the last equation stems from the fact that the restriction of Eq. (51) to  $n \leq 1$  terms gives a truncated expansion in powers of  $\Sigma^2$ . The neglected terms, starting with  $\Sigma^4$ , involve higher derivatives of the density. But having neglected these  $\Sigma^4$  terms, retaining the other  $\Sigma^4$  (and higher) contributions that are summed in  $g(k_{\text{F}} \Sigma)$  is somewhat arbitrary. Therefore, Negele and Vautherin argue that it is advantageous to use this arbitrariness to “reverse engineer” the expansion so that the exact nuclear matter limit is always exactly reproduced by the leading term [33]. We emphasize that this is a prescription without established power counting or error estimates, which must be assessed in future work. As we show in Section 5, different prescriptions can lead to significant changes in nuclear observables.

The gradient terms in the above equation can be evaluated with the aid of the

chain rule<sup>6</sup>

$$\nabla\alpha(\rho) = \nabla\rho\frac{\partial\alpha}{\partial\rho}, \quad \nabla^2\alpha(\rho) = \nabla^2\rho\frac{\partial\alpha}{\partial\rho} + |\nabla\rho|^2\frac{\partial^2\alpha}{\partial\rho^2}. \quad (63)$$

Recalling that we define the local Fermi momentum as  $k_F = (3\pi^2\rho)^{1/3}$ , we can explicitly evaluate the first and second derivatives of  $\alpha$ ,

$$\frac{\partial\alpha}{\partial\rho} = j_0(k_F\Delta), \quad \frac{\partial^2\alpha}{\partial\rho^2} = -\frac{k_F\Delta}{3\rho}j_1(k_F\Delta). \quad (64)$$

Pulling it all together, the product of density matrices in Eq. (38) are approximately given in terms of local quantities by

$$\begin{aligned} \rho(\mathbf{R} + \frac{\mathbf{r}'}{2}, \mathbf{R} + \frac{\mathbf{r}}{2})\rho(\mathbf{R} - \frac{\mathbf{r}'}{2}, \mathbf{R} - \frac{\mathbf{r}}{2}) &\approx \rho_{\text{SL}}^2(k_F\Delta)\rho^2 + \frac{1}{2}\Sigma^2g(k_F\Sigma) \\ &\times \left( \rho\nabla^2\rho\rho_{\text{SL}}(k_F\Delta)j_0(k_F\Delta) - |\nabla\rho|^2[j_0^2(k_F\Delta) + j_1^2(k_F\Delta)] \right) \\ &+ 2\Delta^2g(k_F\Delta)\rho_{\text{SL}}(k_F\Delta)\left( \frac{1}{4}\rho\nabla^2\rho - \rho\tau + \frac{3}{5}k_F^2\rho^2 \right). \end{aligned} \quad (65)$$

### 3.3 Evaluation of $F(\mathbf{R}, \mathbf{q}, \mathbf{p})$ and the DME coupling functions

In the momentum space expression for  $W_{\text{HF}}$ , it remains to evaluate the Fourier transforms defined in Eq. (44) for the expanded density matrices in Eq. (65). Identifying the terms in Eq. (47) that give the DME functionals  $A[\rho]$ ,  $B[\rho]$ , and  $C[\rho]$ , we have

$$F(\mathbf{R}, \mathbf{q}, \mathbf{p})\big|_A = (2\pi)^3\delta(\mathbf{q})\frac{4\pi}{k_F^3}\left[I_1(\bar{p}) + \frac{6}{5}I_2(\bar{p})\right]\rho^2, \quad (66)$$

$$F(\mathbf{R}, \mathbf{q}, \mathbf{p})\big|_B = -(2\pi)^3\delta(\mathbf{q})\frac{8\pi}{k_F^5}I_2(\bar{p})\rho\tau, \quad (67)$$

$$\begin{aligned} F(\mathbf{R}, \mathbf{q}, \mathbf{p})\big|_C &= -\frac{8\pi^2}{k_F^8}I_3(\bar{q})I_5(\bar{p})|\nabla\rho|^2 + \left[(2\pi)^3\delta(\mathbf{q})\frac{2\pi}{k_F^5}I_2(\bar{p}) \right. \\ &\quad \left. + \frac{8\pi^2}{k_F^8}I_3(\bar{q})I_4(\bar{p})\right]\rho\nabla^2\rho, \end{aligned} \quad (68)$$

where  $\bar{p} = p/k_F$  etc., and the  $\mathbf{R}$ -dependence of  $k_F$ ,  $\rho$ , and  $\tau$  has been suppressed. The functions  $I_j(\bar{p})$  and  $I_j(\bar{q})$  are simple polynomials (and theta functions) in the scaled momenta  $\bar{p}$  and  $\bar{q}$ :

<sup>6</sup> Note that the equations here assume the canonical choice of  $k_F = (3\pi^2\rho/2)^{1/3}$ . Alternative choices for  $k_F$ , such as the one proposed by Campi and Bouyssy [61] where  $k_F = k_F(\rho, \nabla^2\rho, \tau)$  will generate additional terms by the chain rule.

$$I_1(\bar{p}) \equiv \int x^2 dx j_0(\bar{p}x) \rho_{\text{SL}}^2(x) = \frac{3\pi}{32} (16 - 12\bar{p} + \bar{p}^3) \theta(2 - \bar{p}) , \quad (69)$$

$$I_2(\bar{p}) \equiv \int x^4 dx j_0(\bar{p}x) \rho_{\text{SL}}(x) g(x) = -\frac{35\pi}{128} (\bar{p}^5 - 18\bar{p}^3 + 40\bar{p}^2 - 24\bar{p}) \theta(2 - \bar{p}) , \quad (70)$$

$$I_3(\bar{q}) \equiv \int x^4 dx j_0(\bar{q}x) g(x) = -\frac{35\pi}{8} (5\bar{q}^2 - 3) \theta(1 - \bar{q}) , \quad (71)$$

$$I_4(\bar{p}) \equiv \int x^2 dx j_0(\bar{p}x) j_0(x) \rho_{\text{SL}}(x) = \frac{3\pi}{8} (2 - \bar{p}) \theta(2 - \bar{p}) , \quad (72)$$

$$I_5(\bar{p}) \equiv \int x^2 dx j_0(\bar{p}x) [j_0^2(x) + j_1^2(x)] = \frac{\pi}{8\bar{p}} (4 - \bar{p}^2) \theta(2 - \bar{p}) . \quad (73)$$

Note that the trivial angular dependence of Eqs. (69)–(73) is a consequence of the angle averaging that is implicit with each application of the DME.

With the aid of Eqs. (66)–(73), we can now obtain explicit expressions for the  $A$ ,  $B$ , and  $C$  coupling functions by grouping terms appropriately and performing the relevant angular integrals. The expressions for  $A$  and  $B$  follow immediately and are given by

$$A[\rho] = \frac{\rho^2}{16\pi k_{\text{F}}^3} \int_0^{2k_{\text{F}}} p^2 dp \text{Tr}_{\sigma\tau}[\tilde{\mathbf{V}}(0, \mathbf{p})] (I_1(\bar{p}) + \frac{6}{5} I_2(\bar{p})) , \quad (74)$$

$$B[\rho] = -\frac{\rho}{8\pi k_{\text{F}}^5} \int_0^{2k_{\text{F}}} p^2 dp \text{Tr}_{\sigma\tau}[\tilde{\mathbf{V}}(0, \mathbf{p})] I_2(\bar{p}) , \quad (75)$$

where  $\text{Tr}_{\sigma\tau}[\tilde{\mathbf{V}}(0, \mathbf{p})]$  is given by a simple sum of diagonal matrix elements in the different partial waves,

$$\text{Tr}_{\sigma\tau}[\tilde{\mathbf{V}}(0, \mathbf{p})] = 8\pi \sum'_{lsj} (2j+1)(2t+1) \langle \frac{p}{2} l s j t | V | \frac{p}{2} l s j t \rangle . \quad (76)$$

The primed sum is over all channels for which  $l + s + t$  is odd.

The contributions to  $W_{\text{HF}}$  that have gradients of the local density take the form

$$W_{\text{HF}}|_{|\nabla\rho|^2} = \int d\mathbf{R} \left( C_{\nabla^2\rho} \nabla^2\rho(\mathbf{R}) + C_{|\nabla\rho|^2} |\nabla\rho(\mathbf{R})|^2 \right) . \quad (77)$$

We can perform a partial integration on the  $\nabla^2\rho$  terms to cast them into the canonical form proportional to only  $|\nabla\rho|^2$ ; that is,

$$W_{\text{HF}}|_{|\nabla\rho|^2} = \int d\mathbf{R} |\nabla\rho(\mathbf{R})|^2 \left[ C_{|\nabla\rho|^2} - \frac{d}{d\rho} C_{\nabla^2\rho} \right] , \quad (78)$$

so that

$$C[\rho] = C_{|\nabla\rho|^2} - \frac{d}{d\rho} C_{\nabla^2\rho} . \quad (79)$$

In practice it is efficient and accurate to calculate the derivative in Eq. (79) numerically rather than analytically.

The expressions for  $C_{|\nabla\rho|^2}$  and  $C_{\nabla^2\rho}$  are obtained by substituting the relevant terms in  $F(\mathbf{R}, \mathbf{q}, \mathbf{p})$  [see Eqs. (66)–(67)] into Eq. (43) and performing the angular integrals,

$$C_{|\nabla\rho|^2} = \frac{1}{32} \int \frac{d\mathbf{q} d\mathbf{p}}{(2\pi)^6} \left( -\frac{8\pi^2}{k_F^8} I_3(\bar{q}) I_5(\bar{p}) \right) \text{Tr}_{\sigma\tau}[\tilde{\mathbf{V}}(\mathbf{q}, \mathbf{p})] \quad (80)$$

$$= -\frac{1}{16\pi^2 k_F^8} \int_0^{k_F} q^2 dq \int_0^{2k_F} p^2 dp I_3(\bar{q}) I_5(\bar{p}) \tilde{\mathbf{V}}_{av}(q, p), \quad (81)$$

$$\begin{aligned} C_{\nabla^2\rho} &= \frac{\rho}{32} \int \frac{d\mathbf{q} d\mathbf{p}}{(2\pi)^6} \left( \frac{1}{k_F^5} (2\pi)^4 \delta^3(\mathbf{q}) I_2(\bar{p}) + \frac{8\pi^2}{k_F^8} I_3(\bar{q}) I_4(\bar{p}) \right) \text{Tr}_{\sigma\tau}[\tilde{\mathbf{V}}(\mathbf{q}, \mathbf{p})] \\ &= \frac{\rho}{32\pi k_F^5} \int_0^{2k_F} p^2 dp I_2(\bar{p}) \text{Tr}_{\sigma\tau}[\tilde{\mathbf{V}}(0, \mathbf{p})] \\ &\quad + \frac{\rho}{16\pi^2 k_F^8} \int_0^{k_F} q^2 dq \int_0^{2k_F} p^2 dp I_3(\bar{q}) I_4(\bar{p}) \tilde{\mathbf{V}}_{av}(q, p), \end{aligned} \quad (82)$$

where  $\tilde{\mathbf{V}}_{av}(q, p)$  is the angle-averaged interaction,

$$\tilde{\mathbf{V}}_{av}(q, p) \equiv \frac{1}{2} \int d(\cos\theta) \text{Tr}_{\sigma\tau}[\tilde{\mathbf{V}}(\mathbf{q}, \mathbf{p})], \quad (83)$$

and  $\tilde{\mathbf{V}}(\mathbf{q}, \mathbf{p})$  is given by Eq. (46). Note that care must be taken in the evaluation of  $dC_{\nabla^2\rho}/d\rho$  if the vertex  $\tilde{\mathbf{V}}(\mathbf{q}, \mathbf{p})$  is density-dependent or if the local Fermi momentum is not taken to be  $k_F = (3\pi^2\rho/2)^{1/3}$ .

## 4 DME for three-body potentials in momentum space

In this section we extend the DME as applied to the Hartree-Fock energy to include three-body force contributions. The low-momentum interactions currently in use do not yet include consistently evolved three-body forces because of technical difficulties in carrying out the momentum-space evolution<sup>7</sup>. Therefore, as an approximation to the evolution, two short-distance low-energy constants in the leading chiral three-body force (this is N<sup>2</sup>LO according to the power counting of Refs. [63,64]) are fit at each cutoff to properties of the

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<sup>7</sup> However, the recent application of similarity renormalization group (SRG) methods to inter-nucleon potentials provide a computationally feasible path to the momentum-space evolution of many-body forces [10,62].

triton and  ${}^4\text{He}$  to determine the three-body force. In the present work, we will use this force exclusively and postpone the treatment of general non-local three-body forces, as will be produced by an SRG evolution.

#### 4.1 $W_{\text{HF}}$ for local three-body forces

The Hartree-Fock 3NF contribution to the total energy is given by

$$W_{\text{HF}}^{(3N)} = \frac{1}{6} \sum_{ijk}^A \langle i j k | V \mathcal{A}_{123} | i j k \rangle , \quad (84)$$

where the summation is over the occupied Kohn-Sham states and the operator  $\mathcal{A}_{123}$  is the (un-normalized) three-nucleon antisymmetrizer

$$\begin{aligned} \mathcal{A}_{123} &= (1 + P_{13}P_{12} + P_{23}P_{12})(1 - P_{12}) \\ &= (1 + P_{13}P_{23} + P_{12}P_{23})(1 - P_{23}) \\ &= (1 + P_{23}P_{13} + P_{12}P_{13})(1 - P_{13}) . \end{aligned} \quad (85)$$

Decomposing the three-body potential in the standard fashion [65],

$$V = V^{(1)} + V^{(2)} + V^{(3)} , \quad (86)$$

where  $V^{(i)}$  is symmetric under  $j \leftrightarrow k$ , we can write the full interaction in terms of one component

$$V = V^{(1)} + P_{23}P_{13}V^{(1)}P_{13}P_{23} + P_{23}P_{12}V^{(1)}P_{12}P_{23} , \quad (87)$$

and so on. This allows us to simplify Eq. (84) by using

$$V \mathcal{A}_{123} = (1 + P_{23}P_{13} + P_{23}P_{12})V^{(1)} \mathcal{A}_{123} , \quad (88)$$

the cyclic nature of the trace along with  $(1 + P_{23}P_{12} + P_{23}P_{13})\mathcal{A}_{123} = 3\mathcal{A}_{123}$ , and other permutation operator identities to obtain

$$\begin{aligned} W_{\text{HF}}^{(3N)} &= \frac{1}{2} \sum_{ijk}^A \langle i j k | V^{(1)} \mathcal{A}_{123} | i j k \rangle \\ &= \frac{1}{2} \sum_{ijk}^A \langle i j k | V^{(1)} (1 + P_{23}P_{12} + P_{13}P_{12} - P_{12} - P_{23} - P_{13}) | i j k \rangle \\ &= \frac{1}{2} \sum_{ijk}^A \langle i j k | V^{(1)} (1 + 2P_{23}P_{12} - 2P_{12} - P_{23}) | i j k \rangle . \end{aligned} \quad (89)$$



Because the leading chiral EFT 3NF has a vanishing direct piece, there are only three independent contributions to  $W_{\text{HF}}$  that need to be evaluated: one double-exchange term involving two permutation operators and two single-exchange contributions. Writing Eq. (89) in terms of density matrices and separating out the scalar-isoscalar contributions to  $W_{\text{HF}}^{(3N)}$  arising from single-exchange terms gives

$$\begin{aligned}
W_{\text{HF}}^{(1x)} &= -\frac{1}{64} \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 \left\{ \right. \\
&\quad \rho(\mathbf{x}_2, \mathbf{x}_1) \rho(\mathbf{x}_1, \mathbf{x}_2) \rho(\mathbf{x}_3) \text{Tr}_{123}[V^{(1)}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) P_{12}^{\sigma\tau}] \\
&\quad \left. + \frac{1}{2} \rho(\mathbf{x}_3, \mathbf{x}_2) \rho(\mathbf{x}_2, \mathbf{x}_3) \rho(\mathbf{x}_1) \text{Tr}_{123}[V^{(1)}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) P_{23}^{\sigma\tau}] \right\} \\
&= -\frac{1}{64} \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 \left\{ \rho(\mathbf{x}_2, \mathbf{x}_1) \rho(\mathbf{x}_1, \mathbf{x}_2) \rho(\mathbf{x}_3) \right. \\
&\quad \times \left( \int \frac{d\mathbf{q}_2 d\mathbf{q}_3}{(2\pi)^6} e^{-i\mathbf{q}_2 \cdot (\mathbf{x}_1 - \mathbf{x}_2)} e^{-i\mathbf{q}_3 \cdot (\mathbf{x}_1 - \mathbf{x}_3)} \text{Tr}_{123}[\tilde{V}^{(1)}(\mathbf{q}_2, \mathbf{q}_3) P_{12}^{\sigma\tau}] \right) \\
&\quad + \frac{1}{2} \rho(\mathbf{x}_3, \mathbf{x}_2) \rho(\mathbf{x}_2, \mathbf{x}_3) \rho(\mathbf{x}_1) \\
&\quad \left. \times \left( \int \frac{d\mathbf{q}_2 d\mathbf{q}_3}{(2\pi)^6} e^{-i\mathbf{q}_2 \cdot (\mathbf{x}_1 - \mathbf{x}_2)} e^{-i\mathbf{q}_3 \cdot (\mathbf{x}_1 - \mathbf{x}_3)} \text{Tr}_{123}[\tilde{V}^{(1)}(\mathbf{q}_2, \mathbf{q}_3) P_{23}^{\sigma\tau}] \right) \right\}, \tag{90}
\end{aligned}$$

where  $\text{Tr}_{123} \equiv \text{Tr}_{\sigma_1\tau_1} \text{Tr}_{\sigma_2\tau_2} \text{Tr}_{\sigma_3\tau_3}$  and a local 3NF has been assumed. Similarly, the scalar-isoscalar contributions to  $W_{\text{HF}}$  arising from the double-exchanges are given by

$$\begin{aligned}
W_{\text{HF}}^{(2x)} &= \frac{1}{64} \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 \rho(\mathbf{x}_1, \mathbf{x}_2) \rho(\mathbf{x}_2, \mathbf{x}_3) \rho(\mathbf{x}_3, \mathbf{x}_1) \left\{ \right. \\
&\quad \left. \int \frac{d\mathbf{q}_2 d\mathbf{q}_3}{(2\pi)^6} e^{-i\mathbf{q}_2 \cdot \mathbf{x}_{12}} e^{-i\mathbf{q}_3 \cdot \mathbf{x}_{13}} \text{Tr}_{123}[\tilde{V}^{(1)}(\mathbf{q}_2, \mathbf{q}_3) P_{23}^{\sigma\tau} P_{12}^{\sigma\tau}] \right\}, \tag{91}
\end{aligned}$$

where the Fourier transformed 3NF components are defined by

$$\langle \mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3 | V^{(1)} | \mathbf{k}'_1 \mathbf{k}'_2 \mathbf{k}'_3 \rangle = \left( \frac{2\pi}{\Omega} \right)^3 \delta(\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3) \tilde{V}^{(1)}(\mathbf{q}_2, \mathbf{q}_3). \tag{92}$$

Here  $\Omega$  is the volume (which drops out of all final expressions) and  $\mathbf{q}_i = \mathbf{k}_i - \mathbf{k}'_i$  is the momentum transfer.

As discussed above, we approximate the RG evolution of the 3N force with the leading-order chiral 3N force, which is comprised of a long-range  $2\pi$ -exchange part  $V_c$ , an intermediate-range  $1\pi$ -exchange part  $V_D$  and a short-range contact

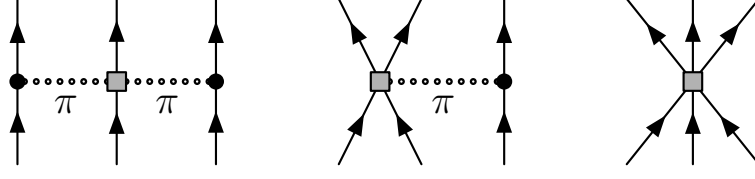


Fig. 3. The chiral three-body force at N<sup>2</sup>LO according to the power counting of Ref. [68], which has a long-range 2 $\pi$ -exchange part  $V_c$  (left), an intermediate-range 1 $\pi$ -exchange part  $V_D$  (middle), and a short-range contact interaction  $V_E$  (right).

interaction  $V_E$  [63,64], see Fig. 3. The 2 $\pi$ -exchange interaction is

$$\tilde{V}_c^{(k)}(\mathbf{q}_i, \mathbf{q}_j) = \left( \frac{g_A}{2f_\pi} \right)^2 \frac{(\boldsymbol{\sigma}_i \cdot \mathbf{q}_i)(\boldsymbol{\sigma}_j \cdot \mathbf{q}_j)}{(q_i^2 + m_\pi^2)(q_j^2 + m_\pi^2)} F_{ijk}^{\alpha\beta} \tau_i^\alpha \tau_j^\beta, \quad (93)$$

where  $F_{ijk}^{\alpha\beta}$  is defined as

$$F_{ijk}^{\alpha\beta} = \delta^{\alpha\beta} \left[ -\frac{4c_1 m_\pi^2}{f_\pi^2} + \frac{2c_3}{f_\pi^2} \mathbf{q}_i \cdot \mathbf{q}_j \right] + \sum_\gamma \frac{c_4}{f_\pi^2} \epsilon^{\alpha\beta\gamma} \tau_k^\gamma \boldsymbol{\sigma}_k \cdot (\mathbf{q}_i \times \mathbf{q}_j), \quad (94)$$

while the 1 $\pi$ -exchange and contact interactions are, respectively,

$$\tilde{V}_D^{(k)}(\mathbf{q}_i, \mathbf{q}_j) = -\frac{g_A}{4f_\pi^2} \frac{c_D}{f_\pi^2 \Lambda_\chi} \frac{\boldsymbol{\sigma}_j \cdot \mathbf{q}_j}{q_j^2 + m_\pi^2} (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j) (\boldsymbol{\sigma}_i \cdot \mathbf{q}_j), \quad (95)$$

$$\tilde{V}_E^{(k)}(\mathbf{q}_i, \mathbf{q}_j) = \frac{c_E}{f_\pi^4 \Lambda_\chi} (\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j). \quad (96)$$

In applying Eqs. (93)–(96), we use  $g_A = 1.29$ ,  $f_\pi = 92.4$  MeV and  $m_\pi = 138.04$  MeV and the  $c_i$  constants extracted by the Nijmegen group in a partial wave analysis with chiral 2 $\pi$ -exchange [66]. These are  $c_1 = -0.76$  GeV<sup>−1</sup>,  $c_3 = -4.78$  GeV<sup>−1</sup> and  $c_4 = 3.96$  GeV<sup>−1</sup>. Fit values for the  $c_D$  and  $c_E$  low-energy constants consistent with a sharply cutoff low-momentum potential are tabulated in Ref. [67] for  $\Lambda_\chi = 700$  MeV.

From the previous general expressions for  $W_{\text{HF}}^{1x}$  and  $W_{\text{HF}}^{2x}$ , we need to evaluate the spin-isospin traces  $\text{Tr}_{123}[\tilde{V}^{(1)} P_{12}^{\sigma\tau}]$ ,  $\text{Tr}_{123}[\tilde{V}^{(1)} P_{23}^{\sigma\tau}]$ , and  $\text{Tr}_{123}[\tilde{V}^{(1)} P_{23}^{\sigma\tau} P_{12}^{\sigma\tau}]$ . For the single-exchanges we find

$$\text{Tr}_{123}[\tilde{V}_E^{(1)}(\mathbf{q}_2, \mathbf{q}_3)P_{23}^{\sigma\tau}] = 48 \frac{c_E}{f_\pi^4 \Lambda_\chi}, \quad (97)$$

$$\text{Tr}_{123}[\tilde{V}_D^{(1)}(\mathbf{q}_2, \mathbf{q}_3)P_{23}^{\sigma\tau}] = -48 \frac{g_A}{4f_\pi^2} \frac{c_D}{f_\pi^2 \Lambda_\chi} \frac{q_3^2}{q_3^2 + m_\pi^2}, \quad (98)$$

$$\begin{aligned} \text{Tr}_{123}[\tilde{V}_c^{(1)}(\mathbf{q}_2, \mathbf{q}_3)P_{23}^{\sigma\tau}] &= 48 \left( \frac{g_A}{2f_\pi} \right)^2 \frac{\mathbf{q}_2 \cdot \mathbf{q}_3}{(q_2^2 + m_\pi^2)(q_3^2 + m_\pi^2)} \\ &\times \left[ -\frac{4c_1 m_\pi^2}{f_\pi^2} + \frac{2c_3}{f_\pi^2} \mathbf{q}_2 \cdot \mathbf{q}_3 \right], \end{aligned} \quad (99)$$

$$\begin{aligned} \text{Tr}_{123}[\tilde{V}_E^{(1)}(\mathbf{q}_2, \mathbf{q}_3)P_{12}^{\sigma\tau}] &= \text{Tr}_{123}[\tilde{V}_D^{(1)}(\mathbf{q}_2, \mathbf{q}_3)P_{12}^{\sigma\tau}] \\ &= \text{Tr}_{123}[\tilde{V}_c^{(1)}(\mathbf{q}_2, \mathbf{q}_3)P_{12}^{\sigma\tau}] = 0, \end{aligned} \quad (100)$$

while the various double-exchange terms give

$$\text{Tr}_{123}[\tilde{V}_E^{(1)}(\mathbf{q}_2, \mathbf{q}_3)P_{23}^{\sigma\tau}P_{12}^{\sigma\tau}] = 12 \frac{c_E}{f_\pi^4 \Lambda_\chi}, \quad (101)$$

$$\text{Tr}_{123}[\tilde{V}_D^{(1)}(\mathbf{q}_2, \mathbf{q}_3)P_{23}^{\sigma\tau}P_{12}^{\sigma\tau}] = -12 \frac{g_A}{4f_\pi^2} \frac{c_D}{f_\pi^2 \Lambda_\chi} \frac{q_3^2}{q_3^2 + m_\pi^2}, \quad (102)$$

$$\begin{aligned} \text{Tr}_{123}[\tilde{V}_c^{(1)}(\mathbf{q}_2, \mathbf{q}_3)P_{23}^{\sigma\tau}P_{12}^{\sigma\tau}] &= 12 \left( \frac{g_A}{2f_\pi} \right)^2 \frac{\mathbf{q}_2 \cdot \mathbf{q}_3}{(q_2^2 + m_\pi^2)(q_3^2 + m_\pi^2)} \\ &\times \left[ -\frac{4c_1 m_\pi^2}{f_\pi^2} + \frac{2c_3}{f_\pi^2} (1 + c_4/c_3) \mathbf{q}_2 \cdot \mathbf{q}_3 \right] \\ &- 24 \left( \frac{g_A}{2f_\pi} \right)^2 \frac{c_4}{f_\pi^2} \frac{q_2^2 q_3^2}{(q_2^2 + m_\pi^2)(q_3^2 + m_\pi^2)}. \end{aligned} \quad (103)$$

Note that for the  $V_E$  and  $V_D$  terms, it is not necessary to treat separately the single- and double-exchange contributions because their structure is identical due to the nature of the zero-range three- and two-body vertices. Substituting the spin-isospin-traced interactions into Eqs. (90)–(91) and simplifying gives

$$W_{\text{HF}}^E = -\frac{3}{16} g_E \int d\mathbf{x} [\rho(\mathbf{x})]^3, \quad (104)$$

$$\begin{aligned} W_{\text{HF}}^D &= \frac{3}{16} g_D \int d\mathbf{x}_2 d\mathbf{x}_3 [\rho(\mathbf{x}_2, \mathbf{x}_3)]^2 \rho(\mathbf{x}_2) \\ &\times \left( \int \frac{d\mathbf{q}_3}{(2\pi)^3} e^{-i\mathbf{q}_3 \cdot (\mathbf{x}_2 - \mathbf{x}_3)} \frac{q_3^2}{q_3^2 + m_\pi^2} \right), \end{aligned} \quad (105)$$

where  $g_E \equiv c_E/f_\pi^4 \Lambda_\chi$  and  $g_D \equiv (g_A/4f_\pi^2)(c_D/f_\pi^2 \Lambda_\chi)$ . Similarly, the single- and double-exchange contributions from the  $2\pi$ -exchange 3NF are given by

$$\begin{aligned}
W_{\text{HF}}^{(1x,c)} = & -\frac{3}{8}g_c \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 \rho(\mathbf{x}_1)\rho(\mathbf{x}_2, \mathbf{x}_3)\rho(\mathbf{x}_3, \mathbf{x}_2) \\
& \times \left\{ \int \frac{d\mathbf{q}_2 d\mathbf{q}_3}{(2\pi)^6} e^{-i\mathbf{q}_2 \cdot (\mathbf{x}_1 - \mathbf{x}_2)} e^{-i\mathbf{q}_3 \cdot (\mathbf{x}_1 - \mathbf{x}_3)} \frac{\mathbf{q}_2 \cdot \mathbf{q}_3}{(q_2^2 + m_\pi^2)(q_3^2 + m_\pi^2)} \right. \\
& \left. \times \left[ -\frac{4c_1 m_\pi^2}{f_\pi^2} + \frac{2c_3}{f_\pi^2} \mathbf{q}_2 \cdot \mathbf{q}_3 \right] \right\}, \tag{106}
\end{aligned}$$

and

$$\begin{aligned}
W_{\text{HF}}^{(2x,c)} = & \frac{3}{16}g_c \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 \rho(\mathbf{x}_1, \mathbf{x}_2)\rho(\mathbf{x}_2, \mathbf{x}_3)\rho(\mathbf{x}_3, \mathbf{x}_1) \\
& \times \int \frac{d\mathbf{q}_2 d\mathbf{q}_3}{(2\pi)^6} e^{-i\mathbf{q}_2 \cdot (\mathbf{x}_1 - \mathbf{x}_2)} e^{-i\mathbf{q}_3 \cdot (\mathbf{x}_1 - \mathbf{x}_3)} \left\{ \frac{\mathbf{q}_2 \cdot \mathbf{q}_3}{(q_2^2 + m_\pi^2)(q_3^2 + m_\pi^2)} \right. \\
& \times \left[ -\frac{4c_1 m_\pi^2}{f_\pi^2} + \frac{2c_3}{f_\pi^2} (1 + c_4/c_3) \mathbf{q}_2 \cdot \mathbf{q}_3 \right] \\
& \left. - \frac{2c_4}{f_\pi^2} \frac{q_2^2 q_3^2}{(q_2^2 + m_\pi^2)(q_3^2 + m_\pi^2)} \right\}, \tag{107}
\end{aligned}$$

where  $g_c \equiv (g_A/2f_\pi)^2$ .

#### 4.2 D-term

As with the nucleon-nucleon contributions to  $W_{\text{HF}}$ , it is convenient to recast the 3NF Hartree-Fock expressions into momentum space. Changing to relative/center-of-mass coordinates ( $\mathbf{R} = (\mathbf{x}_2 + \mathbf{x}_3)/2$ ,  $\mathbf{r} = \mathbf{x}_2 - \mathbf{x}_3$ ), the  $1\pi$ -exchange 3N Hartree-Fock contribution becomes

$$\begin{aligned}
W_{\text{HF}}^D = & \frac{3}{16}g_D \int d\mathbf{R} d\mathbf{r} [\rho(\mathbf{R} + \mathbf{r}/2, \mathbf{R} - \mathbf{r}/2)]^2 \rho(\mathbf{R} + \mathbf{r}/2) \\
& \times \int \frac{d\mathbf{q}}{(2\pi)^3} e^{-i\mathbf{q} \cdot \mathbf{r}} \frac{q^2}{q^2 + m_\pi^2} \\
= & \frac{3}{16}g_D \int d\mathbf{R} \int \frac{d\mathbf{q}}{(2\pi)^3} F(\mathbf{R}, \mathbf{q}) \frac{q^2}{q^2 + m_\pi^2}, \tag{108}
\end{aligned}$$

where we have defined

$$F(\mathbf{R}, \mathbf{q}) \equiv \int d\mathbf{r} e^{-i\mathbf{q} \cdot \mathbf{r}} [\rho(\mathbf{R} + \mathbf{r}/2, \mathbf{R} - \mathbf{r}/2)]^2 \rho(\mathbf{R} + \mathbf{r}/2). \tag{109}$$

Applying the DME separately to the product of non-local and local densities in  $F(\mathbf{R}, \mathbf{q})$  yields

$$[\rho(\mathbf{R} + \mathbf{r}/2, \mathbf{R} - \mathbf{r}/2)]^2 \approx \rho_{\text{SL}}(k_{\text{F}}r)\rho + r^2 g(k_{\text{F}}r) \left[ \frac{1}{2} \rho \nabla^2 \rho - 2\rho\tau + \frac{3}{5} k_{\text{F}}^2 \rho^2 \right], \quad (110)$$

and

$$\rho(\mathbf{R} + \mathbf{r}/2) \approx \rho_{\text{SL}}(k_{\text{F}}r)\rho + r^2 g(k_{\text{F}}r) \left[ \frac{1}{4} \nabla^2 \rho + \frac{3}{5} k_{\text{F}}^2 \rho \right]. \quad (111)$$

Combining the two expansions and dropping terms of higher order in the DME, we find

$$\begin{aligned} [\rho(\mathbf{R} + \mathbf{r}/2, \mathbf{R} - \mathbf{r}/2)]^2 \rho(\mathbf{R} + \mathbf{r}/2) &\approx \rho_{\text{SL}}^2(k_{\text{F}}r)\rho^3 \\ &+ r^2 g(k_{\text{F}}r) \rho_{\text{SL}}(k_{\text{F}}r) \left[ \frac{3}{4} \rho^2 \nabla^2 \rho - 2\rho^2 \tau + \frac{6}{5} k_{\text{F}}^2 \rho^3 \right], \end{aligned} \quad (112)$$

where the  $\mathbf{R}$ -dependence of  $k_{\text{F}}$  and the local densities has been suppressed. Evaluating the Fourier transform defined in Eq. (109) using the approximate DME expressions and grouping terms according to which coupling function contribute gives

$$F(\mathbf{R}, \mathbf{q})|_A = 4\pi \left( \frac{\rho}{k_{\text{F}}} \right)^3 \left[ I_1(\bar{q}) + \frac{6}{5} I_2(\bar{q}) \right], \quad (113)$$

$$F(\mathbf{R}, \mathbf{q})|_B = -\frac{8\pi \rho^2 \tau}{k_{\text{F}}^5} I_2(\bar{q}), \quad (114)$$

$$F(\mathbf{R}, \mathbf{q})|_C = \frac{3\pi}{k_{\text{F}}^5} \rho^2 \nabla^2 \rho I_2(\bar{q}), \quad (115)$$

where the integrals  $I_1(\bar{q})$  and  $I_2(\bar{q})$  were defined in Eqs. (69)–(70) and  $\bar{q} \equiv q/k_{\text{F}}$ . Together with Eq. (108), we obtain the  $1\pi$ -exchange 3NF contributions to the EDF coupling functions

$$A_D[\rho] = \frac{3\rho^3}{8\pi k_{\text{F}}^3} g_D \int dq \frac{q^4}{q^2 + m_{\pi}^2} \left[ I_1(\bar{q}) + \frac{6}{5} I_2(\bar{q}) \right], \quad (116)$$

$$B_D[\rho] = -\frac{3\rho^2}{4\pi k_{\text{F}}^5} g_D \int dq \frac{q^4}{q^2 + m_{\pi}^2} I_2(\bar{q}), \quad (117)$$

$$C_D[\rho] = -\frac{9}{32\pi} g_D \frac{d}{d\rho} \left( \frac{\rho^2}{k_{\text{F}}^5} \int dq \frac{q^4}{q^2 + m_{\pi}^2} I_2(\bar{q}) \right). \quad (118)$$

### 4.3 *c*-term single-exchange

Starting from the single-exchange HF contribution of the  $2\pi$ -exchange 3NF in Eq. (106), we first change to Jacobi coordinates,

$$\mathbf{r}_{23} = \mathbf{x}_2 - \mathbf{x}_3, \quad \mathbf{r}_1 = \mathbf{x}_2 - \frac{1}{2}(\mathbf{x}_3 + \mathbf{x}_1), \quad \mathbf{R} = \frac{1}{3}(\mathbf{x}_1 + \mathbf{x}_2 + \mathbf{x}_3), \quad (119)$$

followed by the change of momentum variables  $\mathbf{q} \equiv \frac{1}{2}(\mathbf{q}_2 - \mathbf{q}_3)$  and  $\mathbf{p} = \mathbf{q}_2 + \mathbf{q}_3$ . The result is

$$W_{\text{HF}}^{(1x,c)} = -\frac{3}{8}g_c \int d\mathbf{R} \int \frac{d\mathbf{q} d\mathbf{p}}{(2\pi)^6} F_{1x}(\mathbf{R}, \mathbf{p}, \mathbf{q}) V_{c_1c_3}(\mathbf{p}, \mathbf{q}), \quad (120)$$

where  $F_{1x}(\mathbf{R}, \mathbf{p}, \mathbf{q})$  is the Fourier transform of the product of density matrices,

$$F_{1x}(\mathbf{R}, \mathbf{p}, \mathbf{q}) = \int d\mathbf{r}_1 d\mathbf{r}_{23} e^{-i\mathbf{p}\cdot\mathbf{r}_1} e^{i\mathbf{q}\cdot\mathbf{r}_{23}} \rho(\mathbf{R} + 2\mathbf{r}_1/3) \times [\rho(\mathbf{R} - \mathbf{r}_1/3 + \mathbf{r}_{23}/2, \mathbf{R} - \mathbf{r}_1/3 - \mathbf{r}_{23}/2)]^2, \quad (121)$$

and  $V_{c_1c_3}(\mathbf{p}, \mathbf{q})$  is defined as

$$V_{c_1c_3}(\mathbf{p}, \mathbf{q}) = \frac{\mathbf{q}_2 \cdot \mathbf{q}_3}{(\mathbf{q}_2^2 + m_\pi^2)(\mathbf{q}_3^2 + m_\pi^2)} \left[ -\frac{4c_1 m_\pi^2}{f_\pi^2} + \frac{2c_3}{f_\pi^2} \mathbf{q}_2 \cdot \mathbf{q}_3 \right], \quad (122)$$

with  $\mathbf{q}_2 = \mathbf{p}/2 + \mathbf{q}$  and  $\mathbf{q}_3 = \mathbf{p}/2 - \mathbf{q}$ .

Referring to Eq. (121), we first expand  $\rho(\mathbf{x}_2, \mathbf{x}_3)$  as

$$\begin{aligned} \rho(\mathbf{x}_2, \mathbf{x}_3) &= \rho(\mathbf{R} - \mathbf{r}_1/3 + \mathbf{r}_{23}/2, \mathbf{R} - \mathbf{r}_1/3 - \mathbf{r}_{23}/2) \\ &\approx \rho_{\text{SL}}(k_{\text{F}}(\mathbf{R}^-)r_{23}) \rho(\mathbf{R}^-) + r_{23}^2 g(k_{\text{F}}(\mathbf{R}^-)r_{23}) \\ &\quad \times \left[ \frac{1}{4} \nabla^2 \rho(\mathbf{R}^-) - \tau(\mathbf{R}^-) + \frac{3}{5} k_{\text{F}}^2(\mathbf{R}^-) \rho(\mathbf{R}^-) \right], \end{aligned} \quad (123)$$

where  $\mathbf{R}^- \equiv \mathbf{R} - \mathbf{r}_1/3$ . Performing a subsequent expansion about  $\mathbf{R}$  gives

$$\begin{aligned} \rho(\mathbf{x}_2, \mathbf{x}_3) &\approx \rho_{\text{SL}}(k_{\text{F}}r_{23}) \rho + r_{23}^2 g(k_{\text{F}}r_{23}) \left[ \frac{1}{4} \nabla^2 \rho - \tau + \frac{3}{5} k_{\text{F}}^2 \rho \right] \\ &\quad + \frac{1}{9} r_{12}^2 g(k_{\text{F}}r_{23}) \nabla^2 (\rho_{\text{SL}}(k_{\text{F}}r_{23}) \rho), \end{aligned} \quad (124)$$

where the second application of the DME has been modified slightly to ensure the leading term is exact in the nuclear matter limit. Similarly, the diagonal density  $\rho(\mathbf{x}_1)$  is expanded as

$$\rho(\mathbf{R} + \frac{2}{3}\mathbf{r}_1) \approx \rho + \frac{4}{9}r_1^2 g(k_F r_1) \nabla^2 \rho . \quad (125)$$

Therefore, to second order in the DME we obtain

$$\begin{aligned} \rho(\mathbf{R} + 2\mathbf{r}_1/3) [\rho(\mathbf{R} - \mathbf{r}_1/3 + \mathbf{r}_{23}/2, \mathbf{R} - \mathbf{r}_1/3 - \mathbf{r}_{23}/2)]^2 &\approx [\rho_{\text{SL}}(k_F r_{23})]^2 \rho^3 \\ &+ 2r_{23}^2 g(k_F r_{23}) \rho_{\text{SL}}(k_F r_{23}) \left[ \frac{1}{4} \rho^2 \nabla^2 \rho - \rho^2 \tau + \frac{3}{5} k_F^2 \rho^3 \right] \\ &+ \frac{1}{9} r_1^2 g(k_F r_1) \nabla^2 (\rho_{\text{SL}}(k_F r_{23}) \rho) + \frac{4}{9} r_1^2 g(k_F r_1) \rho_{\text{SL}}^2(k_F r_{23}) \rho^2 \nabla^2 \rho . \end{aligned} \quad (126)$$

For the usual LDA choice for  $k_F(\mathbf{R})$ , the  $\nabla^2(\rho_{\text{SL}}\rho)$  term evaluates to

$$\begin{aligned} \nabla^2(\rho_{\text{SL}}(k_F r_{23})) &= \left[ \left\{ \rho_{\text{SL}}(k_F r_{23}) + \rho \frac{\partial}{\partial \rho} \rho_{\text{SL}}(k_F r_{23}) \right\} \nabla^2 \rho \right. \\ &\quad \left. + \left\{ 2 \frac{\partial}{\partial \rho} \rho_{\text{SL}}(k_F r_{23}) + \rho \frac{\partial^2}{\partial \rho^2} \rho_{\text{SL}}(k_F r_{23}) \right\} |\nabla \rho|^2 \right] , \end{aligned} \quad (127)$$

which suggests a grouping of terms in Eq. (126) according to which coupling function they contribute to,

$$\rho \cdot \rho^2 \Big|_A = \rho_{\text{SL}}^2(k_F r_{23}) \rho^3 + \frac{6}{5} r_{23}^2 g(k_F r_{23}) \rho_{\text{SL}}(k_F r_{23}) k_F^2 \rho^3 , \quad (128)$$

$$\rho \cdot \rho^2 \Big|_B = -2r_{23}^2 g(k_F r_{23}) \rho_{\text{SL}}(k_F r_{23}) \rho^2 \tau , \quad (129)$$

$$\begin{aligned} \rho \cdot \rho^2 \Big|_C &= \left[ \frac{1}{2} r_{23}^2 g(k_F r_{23}) \rho_{\text{SL}}(k_F r_{23}) \rho^2 + \frac{2}{9} r_1^2 g(k_F r_1) \rho_{\text{SL}}(k_F r_{23}) \rho^2 \right. \\ &\quad \times \left\{ 3 \rho_{\text{SL}}(k_F r_{23}) + \rho \frac{\partial}{\partial \rho} \rho_{\text{SL}}(k_F r_{23}) \right\} \Big] \nabla^2 \rho \\ &\quad + \left[ \frac{2}{9} r_1^2 g(k_F r_1) \rho_{\text{SL}}(k_F r_{23}) \rho^2 \right. \\ &\quad \times \left\{ 2 \frac{\partial}{\partial \rho} \rho_{\text{SL}}(k_F r_{23}) + \rho \frac{\partial^2}{\partial \rho^2} \rho_{\text{SL}}(k_F r_{23}) \right\} \Big] (\nabla \rho)^2 . \end{aligned} \quad (130)$$

Evaluating the Fourier transform in Eq. (121) gives

$$F_{1x}(\mathbf{R}, \mathbf{p}, \mathbf{q}) \Big|_A = (2\pi)^4 \delta(\mathbf{p}) \frac{2\rho^3}{k_F^3} \left[ I_1(\bar{q}) + \frac{6}{5} I_2(\bar{q}) \right] , \quad (131)$$

$$F_{1x}(\mathbf{R}, \mathbf{p}, \mathbf{q}) \Big|_B = -(2\pi)^4 \delta(\mathbf{p}) \frac{4\rho^2 \tau}{k_F^5} I_2(\bar{q}) , \quad (132)$$

$$\begin{aligned} F_{1x}(\mathbf{R}, \mathbf{p}, \mathbf{q}) \Big|_C &= \left[ (2\pi)^4 \delta(\mathbf{p}) \frac{\rho^2}{k_F^5} I_2(\bar{q}) \right. \\ &\quad + \frac{32\pi^2 \rho^2}{3k_F^8} I_3(\bar{p}) \left( I_1(\bar{q}) - \frac{1}{3} I_6(\bar{q}) \right) \Big] \nabla^2 \rho \\ &\quad - \left[ \frac{32\pi^2 \rho}{9k_F^8} I_3(\bar{p}) \left\{ I_6(\bar{q}) + \frac{2}{15} I_7(\bar{q}) - \frac{1}{5} I_8(\bar{q}) \right\} \right] (\nabla \rho)^2 , \end{aligned} \quad (133)$$

where  $I_1$ – $I_5$  have been defined in Eqs. (69)–(73) and the new integrals  $I_6$ – $I_8$  are defined as

$$I_6(\bar{p}) \equiv \int x^2 dx j_0(\bar{p}x) \rho_{\text{SL}}(x) j_2(x) = \frac{3\pi}{32} (8 - 8\bar{p} + \bar{p}^3) \theta(2 - \bar{p}) , \quad (134)$$

$$I_7(\bar{p}) \equiv \int x^3 dx j_0(\bar{p}x) \rho_{\text{SL}}(x) j_1(x) = \frac{3\pi}{8\bar{p}} (2 - \bar{p}^2) \theta(2 - \bar{p}) , \quad (135)$$

$$\begin{aligned} I_8(\bar{p}) &\equiv \int x^3 dx j_0(\bar{p}x) \rho_{\text{SL}}(x) j_3(x) \\ &= \frac{3\pi}{32\bar{p}} (-8 + 40\bar{p} - 36\bar{p}^2 + 5\bar{p}^4) \theta(2 - \bar{p}) . \end{aligned} \quad (136)$$

With explicit expressions for the DME approximation to  $F_{1x}(\mathbf{R}, \mathbf{p}, \mathbf{q})$  in hand, all that remains is to insert Eqs. (131)–(133) into Eq. (120) and group terms accordingly. The  $A[\rho]$  and  $B[\rho]$  coupling functions follow immediately and are given by

$$A[\rho]_{2\pi}^{1x} = -\frac{3g_A^2 \rho^3}{16\pi f_\pi^2 k_F^3} \int q^2 dq V_{c_1 c_3}(0, q) \left[ I_1(\bar{q}) + \frac{6}{5} I_2(\bar{q}) \right] , \quad (137)$$

$$B[\rho]_{2\pi}^{1x} = \frac{3g_A^2 \rho^2}{8\pi f_\pi^2 k_F^5} \int q^2 dq V_{c_1 c_3}(0, q) I_2(\bar{q}) . \quad (138)$$

The derivation of the  $C[\rho]_{2\pi}^{1x}$  coupling is a bit more complicated because we must first partially integrate all  $\nabla^2 \rho$  terms. Writing the gradient contributions to  $W_{\text{HF}}^{1x}$  as

$$\begin{aligned} W_{\text{HF}}^{(1x)} \Big|_{|\nabla \rho|^2} &= \int d\mathbf{R} \left[ C_{\nabla^2 \rho}^{1x} \nabla^2 \rho(\mathbf{R}) + C_{|\nabla \rho|^2}^{1x} |\nabla \rho(\mathbf{R})|^2 \right] \\ &= \int d\mathbf{R} |\nabla \rho(\mathbf{R})|^2 \left[ C_{|\nabla \rho|^2}^{1x} - \frac{d}{d\rho} C_{\nabla^2 \rho}^{1x} \right] , \end{aligned} \quad (139)$$



we obtain

$$C[\rho]_{2\pi}^{1x} = C_{|\nabla\rho|^2}^{1x} - \frac{d}{d\rho} C_{\nabla^2\rho}^{1x} . \quad (140)$$

Comparing to Eqs. (120) and (133) we find

$$\begin{aligned} C_{|\nabla\rho|^2}^{1x} = & -\frac{g_A^2\rho}{12\pi^2 f_\pi^2 k_F^8} \int p^2 dp q^2 dq \bar{V}_{c_1 c_3}(p, q) I_3(\bar{p}) \\ & \times \left\{ -I_6(\bar{q}) - \frac{2}{15} I_7(\bar{q}) + \frac{1}{5} I_8(\bar{q}) \right\} \end{aligned} \quad (141)$$

and

$$\begin{aligned} C_{\nabla^2\rho}^{1x} = & -\frac{3g_A^2\rho^2}{32\pi f_\pi^2 k_F^5} \int q^2 dq V_{c_1 c_3}(0, q) I_2(\bar{q}) \\ & -\frac{g_A^2\rho^2}{4\pi^2 f_\pi^2 k_F^8} \int p^2 dp q^2 dq \bar{V}_{c_1 c_3}(p, q) I_3(\bar{p}) \left\{ I_1(\bar{q}) - \frac{1}{3} I_6(\bar{q}) \right\} , \end{aligned} \quad (142)$$

where the angle-averaged interaction  $\bar{V}_{c_1 c_3}(p, q)$  is defined as

$$\bar{V}_{c_1 c_3}(p, q) \equiv \frac{1}{2} \int d\cos\theta V_{c_1 c_3}(\mathbf{p}, \mathbf{q}) . \quad (143)$$

#### 4.4 *c-term double exchange*

The double exchange contribution from the c-term is given in Eq. (91). Since this involves a product of three off-diagonal density matrices, the DME is significantly more involved than for the other 3N contributions. In order to assess the sensitivity to the details of the (non-unique) DME prescription, we consider two different expansion schemes for these contributions, which we denote by DME I and DME II. We expect the differences between the two schemes should be “small” if the master formula Eq. (53) is indeed a controlled expansion, and if results are insensitive to the different angle-averaging used in the two schemes.

##### 4.4.1 *DME I*

We start by noting that repeated application of the master formula Eq. (53) factorizes the three-body center-of-mass and relative coordinate dependence as

$$\rho(\mathbf{x}_i, \mathbf{x}_j) = \sum_l \lambda_l(r_m, r_{ij}) \mathcal{O}_l(R) . \quad (144)$$

where  $\mathcal{O}_l(R)$  is some monomial of the local densities and  $i, j, m$  are a permutation of 1, 2, and 3. The relative coordinate functions can be written in terms

of their Fourier transforms, e.g.,

$$\tilde{\lambda}(k_m, k_{ij}) = \int \frac{d\mathbf{r}_m d\mathbf{r}_{ij}}{(2\pi)^6} e^{i\mathbf{k}_m \mathbf{r}_m} e^{i\mathbf{k}_{ij} \mathbf{r}_{ij}} \lambda(r_m, r_{ij}) . \quad (145)$$

Expanding the appropriate set of Jacobi coordinates for each density matrix, Eq. (91) can therefore be written as

$$\begin{aligned} W_{\text{HF}}^{(2x,c)} = & \frac{1}{(2\pi)^{18}} \frac{3g_c}{16} \sum_{ijm} \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 d\mathbf{q}_2 d\mathbf{q}_3 \mathcal{D}\mathbf{k} V_{c_1 c_3 c_4}(\mathbf{p}, \mathbf{q}) \\ & \times \tilde{\lambda}_i(k_1, k_{23}) \tilde{\lambda}_j(k_2, k_{13}) \tilde{\lambda}_m(k_3, k_{12}) \mathcal{O}_i(R) \mathcal{O}_j(R) \mathcal{O}_k(R) \\ & \times e^{-i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \mathbf{k}_2 \cdot \mathbf{r}_2 + \mathbf{k}_3 \cdot \mathbf{r}_3 + \mathbf{k}_{13} \cdot \mathbf{r}_{13} + \mathbf{k}_{12} \cdot \mathbf{r}_{12} + \mathbf{k}_{23} \cdot \mathbf{r}_{23} + \mathbf{q}_2 \cdot \mathbf{r}_{12} - \mathbf{q}_3 \cdot \mathbf{r}_{13})} , \end{aligned} \quad (146)$$

with  $g_c = (g_A/2f_\pi)^2$  and where  $\mathcal{D}\mathbf{k}$  denotes an integration over all variables of type  $\mathbf{k}_m$  and  $\mathbf{k}_{ij}$  and

$$\begin{aligned} V_{c_1 c_3 c_4}(\mathbf{p}, \mathbf{q}) = & \frac{\mathbf{q}_2 \cdot \mathbf{q}_3}{(q_2^2 + m_\pi^2)(q_3^2 + m_\pi^2)} \left[ -\frac{4c_1 m_\pi^2}{f_\pi^2} + \frac{2c_3}{f_\pi^2} (1 + c_4/c_3) \mathbf{q}_2 \cdot \mathbf{q}_3 \right] \\ & - 2 \frac{c_4}{f_\pi^2} \frac{q_2^2 q_3^2}{(q_2^2 + m_\pi^2)(q_3^2 + m_\pi^2)} . \end{aligned} \quad (147)$$

Now choose one set of Jacobi coordinates, e.g.,  $\mathbf{r}_2$  and  $\mathbf{r}_{13}$  and rewrite Eq. (146) in terms of these alone

$$\begin{aligned} \mathbf{k}_1 \cdot \mathbf{r}_1 & \longrightarrow \mathbf{k}_1 \cdot \left( -\frac{1}{2}\mathbf{r}_2 - \frac{3}{4}\mathbf{r}_{13} \right) , & \mathbf{k}_{23} \cdot \mathbf{r}_{23} & \longrightarrow \mathbf{k}_{23} \cdot \left( \mathbf{r}_2 - \frac{1}{2}\mathbf{r}_{13} \right) , \\ \mathbf{k}_3 \cdot \mathbf{r}_3 & \longrightarrow \mathbf{k}_3 \cdot \left( -\frac{1}{2}\mathbf{r}_2 + \frac{3}{4}\mathbf{r}_{13} \right) , & \mathbf{k}_{12} \cdot \mathbf{r}_{12} & \longrightarrow \mathbf{k}_{12} \cdot \left( -\mathbf{r}_2 - \frac{1}{2}\mathbf{r}_{13} \right) , \\ \mathbf{q}_2 \cdot \mathbf{r}_{12} & \longrightarrow \mathbf{q}_2 \cdot \left( -\mathbf{r}_2 - \frac{1}{2}\mathbf{r}_{13} \right) . \end{aligned} \quad (148)$$

We obtain as our final result

$$\begin{aligned} W_{\text{HF}}^{(2x,c)} = & \frac{3g_c}{16(2\pi)^{18}} \sum_{i,j,m} \int d\mathbf{R} \mathcal{D}\mathbf{k} \tilde{\lambda}_i(k_1, k_{23}) \tilde{\lambda}_j(k_2, k_{13}) \tilde{\lambda}_m(k_3, k_{12}) \\ & \times \mathcal{O}_i(R) \mathcal{O}_j(R) \mathcal{O}_k(R) V_{c_1 c_3 c_4}(\mathcal{K}_1, \mathcal{K}_2) , \end{aligned} \quad (149)$$

with

$$\begin{aligned} \mathcal{K}_1 & = \mathbf{k}_2 - \frac{1}{2}\mathbf{k}_1 - \frac{1}{2}\mathbf{k}_3 + \mathbf{k}_{23} - \mathbf{k}_{12} , \\ \mathcal{K}_2 & = \mathbf{k}_{13} - \frac{1}{2}\mathbf{k}_1 + \mathbf{k}_3 - \mathbf{k}_{23} . \end{aligned} \quad (150)$$

Now let us consider the particular form of the functions appearing in the integrals. We expand each density matrix as in Eq. (124) and use Eq. (64) to evaluate the  $\nabla^2(\rho_{SL}\rho)$  term:

$$\begin{aligned}\rho(\mathbf{x}_1, \mathbf{x}_2) \approx & \rho \left[ \rho_{SL}(k_F r_{12}) + r_{12}^2 g(k_F r_{12}) \frac{3}{5} k_F^2 \right] + \tau \left[ -r_{12}^2 g(k_F r_{12}) \right] \\ & + \nabla^2 \rho \left[ \frac{r_3^2}{9} g(k_F r_3) j_0(k_F r_{12}) + \frac{r_{12}^2}{4} g(k_F r_{12}) \right] \\ & + |\nabla \rho|^2 \left[ -\frac{r_3^2}{9} g(k_F r_3) \frac{(k_F r_{12})^2}{9\rho} \rho_{SL}(k_F r_{12}) \right].\end{aligned}\quad (151)$$

This leads us to define

$$\lambda_1(r_3, r_{12}) \equiv \left( \rho_{SL}(k_F r_{12}) + r_{12}^2 g(k_F r_{12}) \frac{3}{5} k_F^2 \right), \quad (152)$$

$$\lambda_2(r_3, r_{12}) \equiv -r_{12}^2 g(k_F r_{12}), \quad (153)$$

$$\lambda_3(r_3, r_{12}) \equiv \frac{r_3^2}{9} g(k_F r_3) j_0(k_F r_{12}) + \frac{r_{12}^2}{4} g(k_F r_{12}), \quad (154)$$

$$\lambda_4(r_3, r_{12}) \equiv -\frac{r_3^2}{9} g(k_F r_3) \frac{(k_F r_{12})^2}{9\rho} \rho_{SL}(k_F r_{12}). \quad (155)$$

We obtain the A-term by inserting the relevant functions into Eq. (149)

$$A[\rho] = \frac{3g_c \rho^3}{16(2\pi)^{18}} \int \mathcal{D}\mathbf{k} \tilde{\lambda}_1(k_3, k_{12}) \tilde{\lambda}_1(k_2, k_{13}) \tilde{\lambda}_1(k_1, k_{23}) V_{c_1 c_3 c_4}(\mathcal{K}_1, \mathcal{K}_2), \quad (156)$$

with

$$\begin{aligned}\tilde{\lambda}_1(k_3, k_{12}) &= \left( \frac{6\pi^2}{k_F^3} + \frac{21\pi^2}{2k_F^5} (3k_F^2 - 5k_{12}^2) \right) \Theta(k_F - k_{12}) (2\pi)^3 \delta^{(3)}(\mathbf{k}_3) \\ &= \tilde{\lambda}_1(k_{12}) (2\pi)^3 \delta^{(3)}(\mathbf{k}_3).\end{aligned}\quad (157)$$

Integrating over the  $\delta$ -functions leads to

$$\begin{aligned}A[\rho] &= \frac{3g_c \rho^3}{16(2\pi)^9} \int d\mathbf{k}_{12} d\mathbf{k}_{13} d\mathbf{k}_{23} \tilde{\lambda}_1(k_{12}) \tilde{\lambda}_1(k_{13}) \tilde{\lambda}_1(k_{23}) \\ &\quad \times V_{c_1 c_3 c_4}(\mathbf{k}_{23} - \mathbf{k}_{12}, \mathbf{k}_{13} - \mathbf{k}_{23}).\end{aligned}\quad (158)$$

The B-term is proportional to  $\tau$

$$B[\rho] = \frac{3g_c \rho^2}{16(2\pi)^{18}} \int \mathcal{D}\mathbf{k} V_{c_1 c_3 c_4}(\mathcal{K}_1, \mathcal{K}_2) \left( \tilde{\lambda}_2(k_3, k_{12}) \tilde{\lambda}_1(k_2, k_{13}) \tilde{\lambda}_1(k_1, k_{23}) \right. \\ \left. + \tilde{\lambda}_1(k_3, k_{12}) \tilde{\lambda}_2(k_2, k_{13}) \tilde{\lambda}_1(k_1, k_{23}) + \tilde{\lambda}_1(k_3, k_{12}) \tilde{\lambda}_1(k_2, k_{13}) \tilde{\lambda}_2(k_1, k_{23}) \right) , \quad (159)$$

with

$$\tilde{\lambda}_2(k_3, k_{12}) = -\frac{35\pi^2}{2k_F^7} (3k_F^2 - 5k_{12}^2) \Theta(k_F - k_{12}) (2\pi)^3 \delta^{(3)}(\mathbf{k}_3) \\ = \tilde{\lambda}_2(k_{12}) (2\pi)^3 \delta^{(3)}(\mathbf{k}_3) . \quad (160)$$

Integrating out the  $\delta$ -functions gives

$$B[\rho] = \frac{3g_c \rho^2}{16(2\pi)^9} \int d\mathbf{k}_{12} d\mathbf{k}_{13} d\mathbf{k}_{23} V_{c_1 c_3 c_4}(\mathbf{k}_{23} - \mathbf{k}_{12}, \mathbf{k}_{13} - \mathbf{k}_{23}) \\ \times \left( \tilde{\lambda}_2(k_{12}) \tilde{\lambda}_1(k_{13}) \tilde{\lambda}_1(k_{23}) + \tilde{\lambda}_1(k_{12}) \tilde{\lambda}_2(k_{13}) \tilde{\lambda}_1(k_{23}) \right. \\ \left. + \tilde{\lambda}_1(k_{12}) \tilde{\lambda}_1(k_{13}) \tilde{\lambda}_2(k_{23}) \right) , \quad (161)$$

The calculation of the relevant integrals for the  $C$ -term is more involved. We first consider on the integral for the coefficient of  $|\nabla\rho|^2$

$$C_{|\nabla\rho|^2} = \frac{3g_c \rho^2}{16(2\pi)^{18}} \int \mathcal{D}\mathbf{k} V_{c_1 c_3 c_4}(\mathcal{K}_1, \mathcal{K}_2) \left( \tilde{\lambda}_1(k_3, k_{12}) \tilde{\lambda}_1(k_2, k_{13}) \tilde{\lambda}_4(k_1, k_{23}) \right. \\ \left. + \tilde{\lambda}_1(k_1, k_{23}) \tilde{\lambda}_1(k_2, k_{13}) \tilde{\lambda}_4(k_3, k_{12}) + \tilde{\lambda}_1(k_1, k_{23}) \tilde{\lambda}_1(k_3, k_{12}) \tilde{\lambda}_4(k_2, k_{13}) \right) , \quad (162)$$

with

$$\tilde{\lambda}_4(k_1, k_{23}) = -\frac{35\pi^4}{81\rho k_F^7} (3k_F^2 - 5k_1^2) \Theta(k_F - k_1) \\ \times \left( \frac{1}{k_F k_{23}} \delta(k_F - k_{23}) + \frac{1}{k_{23}} \frac{d}{dk_{23}} \delta(k_F - k_{23}) \right) . \quad (163)$$

Let us focus our attention on the first term in Eq. (162). This term contains a factor

$$\left( \frac{1}{k_F} \delta(k_F - k_{23}) + \frac{d}{dk_{23}} \delta(k_F - k_{23}) \right) \frac{1}{k_{23}} V_{c_1 c_3 c_4} , \quad (164)$$

which simplifies to

$$\frac{2}{k_{23}k_F}\delta(k_F - k_{23})V_{2X} - \frac{1}{k_{23}}\delta(k_F - k_{23})\frac{d}{dk_{23}}V_{2X} . \quad (165)$$

after partial integration.

The second term has the coefficient  $\nabla^2\rho$

$$\begin{aligned} C_{\nabla^2\rho} = & \frac{3g_c\rho^2}{16(2\pi)^{18}} \int \mathcal{D}^3k V_{c_1c_3c_4}(\mathcal{K}_1, \mathcal{K}_2) \Big( \tilde{\lambda}_1(k_3, k_{12})\tilde{\lambda}_1(k_2, k_{13})\tilde{\lambda}_3(k_1, k_{23}) \\ & + \tilde{\lambda}_1(k_1, k_{23})\tilde{\lambda}_1(k_2, k_{13})\tilde{\lambda}_3(k_3, k_{12}) + \tilde{\lambda}_1(k_1, k_{23})\tilde{\lambda}_1(k_3, k_{12})\tilde{\lambda}_3(k_2, k_{13}) \Big) , \end{aligned} \quad (166)$$

with

$$\begin{aligned} \tilde{\lambda}_3(k_1, k_{23}) = & \frac{35\pi^4}{9k_F^8k_{23}}(3k_F^2 - 5k_1^2)\delta(k_F - k_{23})\Theta(k_F - k_1) \\ & + \frac{35\pi^5}{k_F^7}\delta^{(3)}(\mathbf{k}_1)(3k_F^2 - 5k_{23}^2)\Theta(k_F - k_{23}) \\ = & \lambda_{3A}(k_1)\frac{1}{k_{23}}\delta(k_F - k_{23}) + \lambda_{3B}(k_{23})(2\pi)^3\delta(\mathbf{k}_1) . \end{aligned} \quad (167)$$

Integrating over the  $\delta$ -functions leads to a lengthy expression that we will not give here.

Using partial integration we can finally write the total expression in the form

$$C[\rho] = C_{|\nabla\rho|^2} - \frac{d}{d\rho}C_{\nabla^2\rho} . \quad (168)$$

The particular order of integrations we have carried out gives factors of  $k_F$  appearing as UV cutoffs in the remaining integrals. Such a simplification arises for all contributions to the HF energy and the resulting integrals can therefore be easily integrated numerically despite the relatively large number of integration variables.

Key to the prescription used here is the Fourier transform of the expanded density matrices to momentum space. Due to its generality, this approach can easily be extended to the calculation of higher-order contributions to the DME. A similar approach was introduced in Ref. [45], where the authors used the Fourier transform of the expanded density matrix to generate medium insertions for a diagrammatic calculation of the nuclear energy density functional using chiral perturbation theory.

#### 4.4.2 DME II

The DME I prescription outlined above differs from the original NV approach in two respects. First, we do not rearrange and truncate the expansion by hand to ensure that the nuclear matter limit is exactly reproduced. Second, the DME I prescription keeps cross-terms in the product of the three expanded density matrices that are formally of higher order in the NV approach. In order to quantify these effects and assess whether the expansion is under control, we have also performed the expansion where we strictly follow the original NV philosophy (DME II).

We also note the differences in angle-averaging that arise with the different DME schemes. In the DME I approach, each  $\rho(\mathbf{x}_i, \mathbf{x}_j)$  is first expanded in the natural Jacobi coordinates  $(\mathbf{R}, \mathbf{r}_k, \mathbf{r}_{ij})$ , and then the three expanded density matrices are expressed in one common set of Jacobi coordinates. In the DME II prescription, we follow a different path by expressing the product of density matrices in one common set of Jacobi coordinates from the outset. The subsequent DME implies a different angle-averaging, since only one density matrix is expanded in its natural Jacobi basis. We do not include the derivation of the DME II equations here, as it proceeds in much the same spirit as for the DME I, although we note that the final expressions are considerably more cumbersome since one finds different  $\tilde{\lambda}_l$  functions depending on whether one is expanding the  $\rho(\mathbf{x}_i, \mathbf{x}_j)$  corresponding to the chosen Jacobi coordinates or one of the other two density matrices.

## 5 Results

In this section, we make some basic tests of the DME. We have two modest goals: to check that the DME does not degrade when applied to non-local, low-momentum NN potentials and to make a first assessment of the relative contributions of two- and three-body interactions. For the first goal, we approximate the self-consistent Hartree-Fock ground-state wave function by a Slater determinant of harmonic oscillator single-particle wave functions. Using these wave functions, we compare the DME approximation for the energy of a schematic model NN potential to the exact result where the finite range and non-locality of the interaction is treated without approximation. Then with the same wave function we check the error as we change the resolution (cutoff) of a realistic low-momentum potential. For the second goal, we exhibit some numerical results for the DME coefficient functions to illustrate the non-trivial density dependence and to show the effects of different prescriptions for the three-body DME. These are meant only to set a baseline because, at a minimum, we should include second-order contributions (i.e., beyond Hartree-Fock) before expecting quantitative predictions for nuclear

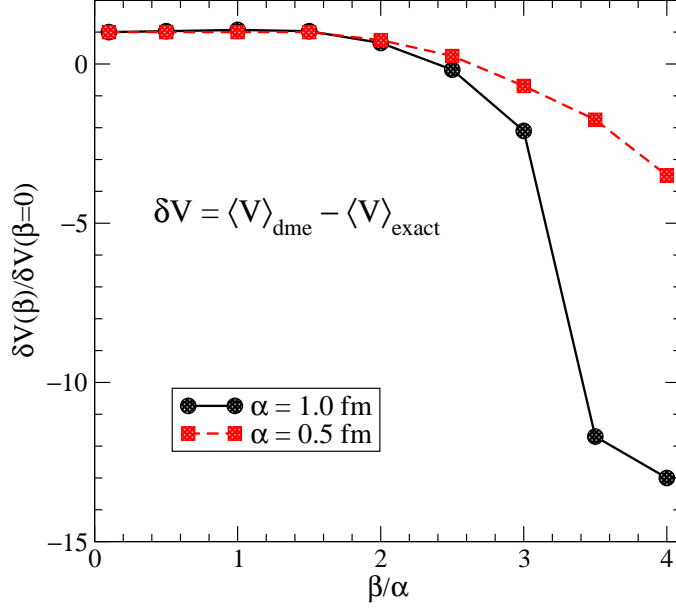


Fig. 4. Effects of different non-localities on the accuracy of the DME as a function of the ratio of the non-locality to range parameters for the harmonic oscillator approximation to the ground state of  $^{40}\text{Ca}$ .

structure or analyzing the cutoff dependence of the energy functional. However, even at this stage it should be meaningful to use these results to compare the relative contributions of two- and three-body interactions.

Although the original DME paper introduced formalism for non-local potentials [33], previous investigations of the effectiveness of the DME studied only local potentials (or local approximations to the G matrix). Because the low-momentum potentials used here can be strongly non-local, we first test whether the extra expansion required degrades the accuracy of the DME. We consider a model potential:

$$V(\mathbf{r}, \mathbf{r}') = v\left(\frac{\mathbf{r} + \mathbf{r}'}{2\alpha}\right) \frac{1}{(\pi\beta^2)^{3/2}} e^{-(\mathbf{r}-\mathbf{r}')^2/\beta^2}, \quad (169)$$

with  $v$  a Gaussian potential, so the range is set by  $\alpha$ . The range of the non-locality is set by  $\beta$ ; in the limit  $\beta \rightarrow 0$ ,  $V(\mathbf{r}, \mathbf{r}') \rightarrow v(\mathbf{r}/\alpha)\delta^3(\mathbf{r} - \mathbf{r}')$ .

In Fig. 4, the effects of non-localities on the accuracy of the DME for integrated quantities (e.g.,  $\langle V \rangle$ ) is illustrated using this potential. We use a harmonic oscillator model of  $^{40}\text{Ca}$  (i.e., the ground-state wave function is a Slater determinant of harmonic oscillator orbitals) and calculate the expectation value of the non-local  $V(\mathbf{r}, \mathbf{r}')$  in the Hartree-Fock ground state. For a given range  $\alpha$ , we compare the error for a non-locality  $\beta$  to the error with  $\beta = 0$ . It is evident that the effect of the non-locality on the degradation of the DME is unimportant up to at least twice the range. Even when  $\alpha$  is taken as small as the typical range of a repulsive core there should be no problem

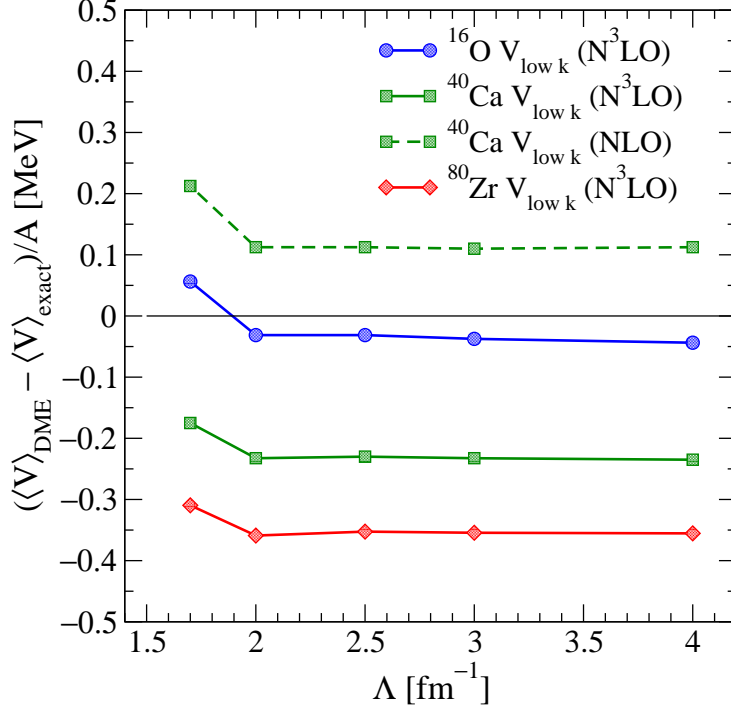


Fig. 5. Errors per nucleon in the DME predictions for the expectation value of a model potential, Eq. (169), in a harmonic oscillator ground state for three  $N = Z$  nuclei (no Coulomb interaction).

for the range of low-momentum cutoffs typically considered.

The errors per nucleon for the DME with the same model ground state but with a realistic low-momentum nucleon-nucleon potential (starting from the chiral N $^3$ LO potential from Ref. [69]) are shown in Fig. 5 for  $N = Z$  nuclei (without Coulomb) for  $A = 16, 40$ , and  $80$ . It is evident that the cutoff dependence of the error is very slight until  $\Lambda < 2 \text{ fm}^{-1}$ . Because the evolution of the potential does not alter the long-distance part, the weak cutoff dependence of the error implies that the short-distance contribution is very well reproduced and provides further confirmation that non-locality (which grows with decreasing  $\Lambda$ ) is not a problem for the DME (note that long-range local interactions remain local). These errors are also smaller than errors found in early DME tests.

The model calculations in Fig. 5 treat both direct (Hartree) and exchange terms with the DME. It was recognized long ago that the DME is ill-suited for long-range direct terms, which should be calculated exactly instead [34]. The dashed line in the figure shows the error for  $A = 40$  but using the NLO potential, which does not have any long-range contributions to the direct scalar term. As expected, the error is significantly smaller than the N $^3$ LO result, due at least in part to the crude treatment of the N $^3$ LO long-range direct contribution. Since the long-range local terms can be isolated in the poten-



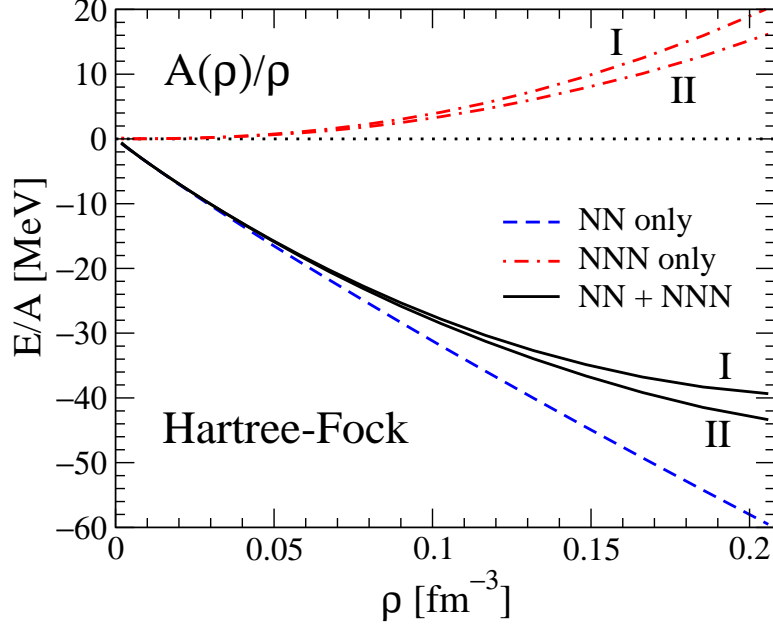


Fig. 6. Contribution to the energy per particle in nuclear matter from the isoscalar coefficient function  $A(\rho)$  as a function of the density from the DME applied to the Hartree-Fock energy calculated using  $V_{\text{low } k}$  with  $\Lambda = 2.1 \text{ fm}^{-1}$ . The result including the NN interaction alone is compared to NN plus NNN interactions for two DME expansions (I and II, see text).

tial, it is feasible to perform exact Hartree evaluations of these pieces when implemented in a DFT solver.

We turn now to the isoscalar  $A$  and  $B$  functions, which are the only contributors to uniform, symmetric nuclear matter. The energy per particle as a function of density  $\rho$  is given by:

$$E/A = \frac{1}{\rho} \left[ \frac{\hbar^2}{2M} \tau + A(\rho) + B(\rho) \tau \right]. \quad (170)$$

The individual contributions from  $A$  and  $B$  at the Hartree-Fock level are plotted in Figs. 6 and 7, and combined into  $E/A$  in Fig. 8. These use a two-body  $V_{\text{low } k}$  interaction evolved from the Argonne  $v_{18}$  potential [70] with a sharp cutoff at  $\Lambda = 2.1 \text{ fm}^{-1}$  and a chiral  $\text{N}^2\text{LO}$  three-body force with constants fit to the binding energies of the triton and  ${}^4\text{He}$  [67]. Results are given using the NN contribution only and with NNN included, using the two prescriptions for the NNN double-exchange contribution (DME-I and DME-II) described in Section 4.

From Figs. 6 and 7, one sees that the ratios of contributions from three-body to two-body tend to increase monotonically with density, but are still only about 20–30% at saturation density. This is consistent with general expectations from chiral power counting. The actual scaling with density of the ratio varies only slightly from being linear in the density. Because the local density in

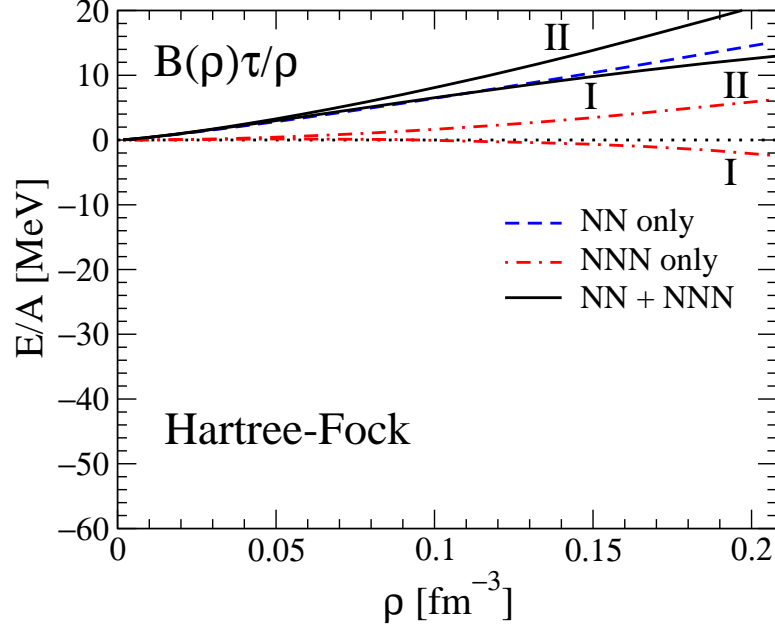


Fig. 7. Contribution to the energy per particle in nuclear matter from the isoscalar coefficient function  $B(\rho)$  as a function of the density from the DME applied to the Hartree-Fock energy calculated using  $V_{\text{low } k}$  with  $\Lambda = 2.1 \text{ fm}^{-1}$ . The result including the NN interaction alone is compared to NN plus NNN interactions for two DME expansions (I and II, see text).

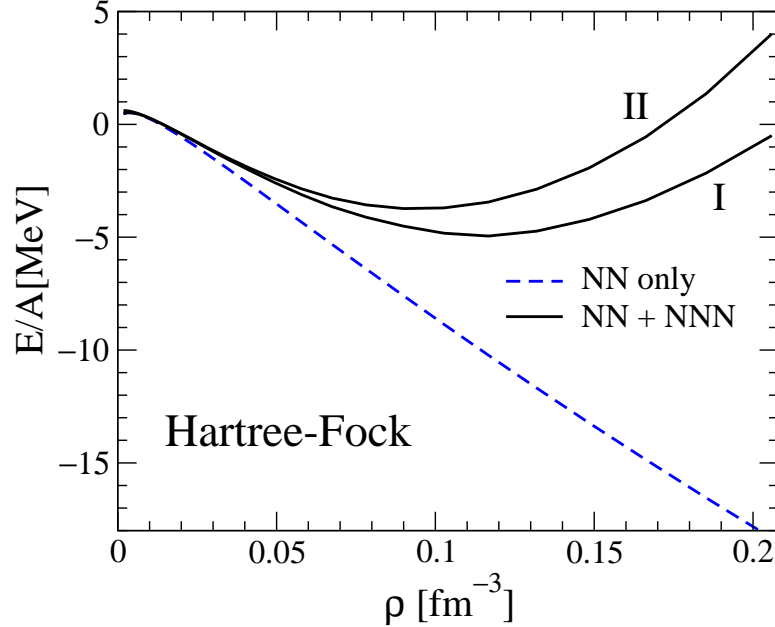


Fig. 8. Energy per particle in nuclear matter by combining contributions from the isoscalar coefficient functions  $A(\rho)$  and  $B(\rho)$  with the kinetic energy as a function of the density from the DME applied to the Hartree-Fock energy calculated using  $V_{\text{low } k}$  with  $\Lambda = 2.1 \text{ fm}^{-1}$ . The result including the NN interaction alone is compared to NN plus NNN interactions for two DME expansions (I and II, see text). Note that only expansion II correctly reproduces the nuclear matter limit.

actual nuclei in somewhat lower, there is reason to believe the expansion in many-body forces is under control. Past estimates of contributions to Skyrme energy functionals based on naive dimensional analysis [71] suggested large contributions from three-body and even four-body interactions. The present results imply more modest contributions, but evaluating the chiral N3LO four-body contribution at Hartree-Fock will be needed for a definitive assessment.

The comparison of the DME-I and DME-II curves gives us an estimate of the truncation error in the expansion applied to the NNN terms because these prescriptions differ in the contributions of higher-order terms in the expansion. Indeed, we have verified that suppressing these terms by hand brings the predictions for the  $A$  and  $B$  coefficients into agreement. The qualitative difference for the NNN-only contribution to  $B$  is large, but the actual coefficient itself is small, so this should not be alarming. However, because the combination of  $A$  and  $B$  and the kinetic energy to obtain the nuclear matter energy per particle involves strong cancellations, the spread in Fig. 8 is large on the scale of nuclear binding energies.

These differences motivate a generalization of the Negele-Vautherin DME following the discussion in Ref. [72]. In this approach, the expansion of the scalar density matrix takes the factorized form

$$\rho(\mathbf{R} + \frac{\mathbf{s}}{2}, \mathbf{R} - \frac{\mathbf{s}}{2}) = \sum_n \Pi_n(k_F s) \langle \mathcal{O}_n(\mathbf{R}) \rangle, \quad (171)$$

where

$$\langle \mathcal{O}_n(\mathbf{R}) \rangle = \{\rho(\mathbf{R}), \tau(\mathbf{R}), \nabla^2 \rho(\mathbf{R}), \dots\}, \quad (172)$$

and  $k_F$  is a momentum scale typically taken to be  $k_F(\mathbf{R})$  as in Eq. (52). Similar expansions are made for the other components of the density matrix. Input from finite nuclei can be used to determine the  $\Pi_n$  functions, which can be viewed as general resummations of the DME expansion; see Section 6 for a brief overview.

Finally, in Fig. 9, the coefficient function  $C(\rho)$  is plotted as a function of density ( $\rho = 2k_F^3/3\pi^2$ ). Even at the highest density, the three-body contribution is a manageable correction to the two-body result. The NN + NNN result is in qualitative agreement with the results of Fritsch and collaborators who included two-pion exchanges with explicit  $\Delta$ -isobars [47], although the three-body contributions in the current work are somewhat larger than effects arising from explicit  $\Delta$ -isobars. For this coefficient function the difference between DME-I and DME-II is comparatively small.

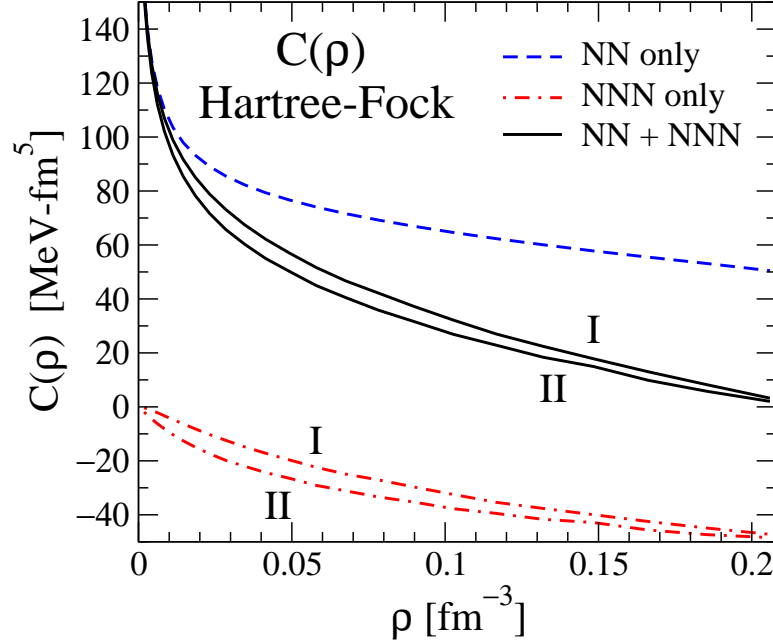


Fig. 9. Isoscalar coefficient function  $C(\rho)$  as a function of the density from the DME applied to the Hartree-Fock energy calculated using  $V_{\text{low } k}$  with  $\Lambda = 2.1 \text{ fm}^{-1}$ . The result including the NN interaction alone is compared to NN plus NNN interactions for two DME expansions (I and II, see text).

## 6 Summary

In this paper, we have formulated the density matrix expansion (DME) for low-momentum interactions and applied it to a Hartree-Fock energy functional including both NN and NNN potentials. The output is a set of functions of density that can replace density-independent parameters in standard Skyrme Hartree-Fock energy density functionals. This replacement in Skyrme HF computer codes is shown schematically in Fig. 10. Only one section of such a code would be replaced, and it takes the same inputs (single-particle eigenvalues and wave functions for the orbitals and the corresponding occupation numbers) and delivers the same outputs (local Kohn-Sham potentials). Furthermore, the upgrade from Skyrme energy functional to DME energy functional can be carried out in stages. For example, the spin-orbit part and pairing can be kept in Skyrme form with the rest given by the DME. Details of such a DME implementation will be given elsewhere. A further upgrade to orbital-based methods would also only modify the same part of the code, although the increased computational load will be significant.

The numerical results given here are limited and do not touch on many of the most interesting aspects of microscopic DFT from low-momentum potentials. Topics to explore in the future include:

- Examine the resolution or scale dependence of the energy functional by

evolving the input low-momentum potential. There will be dependence on the cutoff  $\Lambda$  (if using  $V_{\text{low } k}$ ) or the flow parameter  $\lambda$  (if using  $V_{\text{srg}}$ ) both from omitted physics and from intrinsic scale dependence. Calculations at least to second order are needed to separate these dependencies.

- Examine the isovector part of the functional. We can isolate the contributions from the more interesting long-range (pion) parts of the free-space interactions, allowing us to obtain analytic expressions for the dominant density dependence of the isovector DME coupling functions.
- Study the dependence of spin-orbit contributions on NN vs. NNN interactions. This includes the isospin dependence as well as overall magnitudes. The NN spin-orbit contributions arise from short-range interactions, whereas NNN contributions arise from the long-range two-pion exchange interaction. Therefore, we expect to find a rather different density dependence for the two types of spin-orbit contributions.
- Explore the contribution of tensor contributions, which have recently been reconsidered phenomenologically [73,74].
- Understand the scaling of contributions from many-body forces. In particular, how does the four-body force (which is known at N<sup>3</sup>LO in chiral EFT with conventional Weinberg counting) contribution at Hartree-Fock level impact the energy functional?

The calculations presented here are only the first step on the road to a universal nuclear energy density functional (UNEDF) [15]. There are both refinements within the DME framework and generalizations that test its applicability and accuracy. While many of these steps offer significant challenges, in every case a plan is in hand to carry it out. The DME can be directly extended to include second-order (or full particle-particle ladder) contributions by using averaged energies for the energy denominators. However, a more systematic approximation is under development using a short-time expansion [75]. More difficult future steps include dealing with symmetry breaking and restoration in DFT for self-bound systems, dealing with non-localities from near-on-shell particle-hole excitations (vibrations), and incorporating pairing in the same

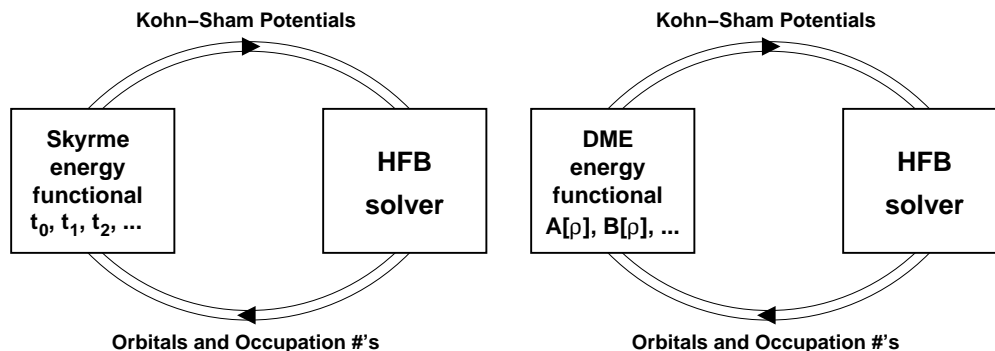


Fig. 10. Diagrams showing the flow in Skyrme HF codes at present (left) and modified for the DME (right).

microscopic framework (see Ref. [41]).

In extending our calculations we will also modify the standard DME formalism from Ref. [33] that we have followed in the present work. The formalism has problems even beyond the truncation errors from different DME prescriptions already discussed in Sections 4 and 5, the most severe being that it provides an extremely poor description of the vector part of the density matrix. While the standard DME is better at reproducing the scalar density matrices, even here the errors are sufficiently large that the disagreement with a full finite-range Hartree-Fock calculations can reach the MeV per particle level. Gebremariam and collaborators have traced both of these problems to an inadequate phase space averaging (PSA) used in the previous DME approaches [39]. In the derivation of the DME, one incorporates average information about the local momentum distribution into the approximation. The Negele-Vautherin DME uses the phase space of infinite nuclear matter to perform this averaging. However, the local momentum distribution in finite Fermi systems exhibits two striking differences from that of infinite homogenous matter. First, mean-field calculations of nuclei show that the local momentum distribution exhibits a diffuse Fermi surface that is especially pronounced in the nuclear surface. Second, the local momentum distribution is found to be anisotropic, with the deformation accentuated in the surface region of the finite Fermi system.

To incorporate both of these missing effects into the DME, Gebremariam et al. have constructed a model for the local momentum distribution based on previous studies of the Wigner distribution function in nuclei [39]. The model parameters are adjusted so that the DME accurately reproduces both integrated quantities, such as the expectation value of the finite-range nucleon-nucleon interaction taken between Slater determinants from self-consistent Skyrme-Hartree-Fock calculations, as well as the density matrices themselves. The improvements are substantial, typically reducing relative errors in integrated quantities by as much as an order of magnitude across many different isotope chains. The improvement is especially striking for the vector density matrices. We will test this improved DME in future investigations.

The tests of the DME will include benchmarks against *ab initio* methods in the overlap region of light-to-medium nuclei. Additional information is obtained from putting the nuclei in external fields, which can be added directly to the DFT/DME functional. Work is in progress on comparisons to both coupled cluster and full configuration interaction calculations. A key feature is that we use the same Hamiltonian for the microscopic calculation and the DME approximation to the DFT. The freedom to adjust (or turn off) external fields as well as to vary other parameters in the Hamiltonian permits detailed evaluations of the approximate functionals. In parallel there will be refined nuclear matter calculations; power counting arguments from re-examining the Brueckner-Bethe-Goldstone approach in light of low-momentum potentials

will provide a framework for organizing higher-order contributions. These investigations should provide insight into how the energy density functional can be fine tuned for greater accuracy in a manner consistent with power counting and EFT principles.

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